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THE APPLICATION OF FINITE ELEMENTS AND
SPACE-ANGLE SYNTHESIS TO THE
ANISOTROPIC STEADY STATE BOLTZMANN
(TRANSPORT) EQUATION

THESIS

AFIT/GNE/PH/81-13   Eze E. Wills
2nd Lt. USAF

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AFIT/GNE/PH/81-13

THE APPLICATION OF FINITE ELEMENTS AND SPACE-ANGLE SYNTHESIS TO THE ANISOTROPIC STEADY STATE BOLTZMANN (TRANSPORT) EQUATION

THESIS

Presented to the Faculty of the School of Engineering
of the Air Force Institute of Technology
Air University
in Partial Fulfillment of the
Requirements for the Degree of
Master of Science

X

by

Eze E. Wills, B.S.
2nd Lt. USAF
Graduate Nuclear Engineering

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Preface

This research project is a part of the ongoing effort here at the Air Force Institute of Technology to develop alternate methods for solving the two-dimensional steady state anisotropic neutral particle transport equation. The thrust of this research effort is towards an accurate and cost-effective solution of the steady state transport of neutrons, gamma rays and high energy x-rays from a low altitude nuclear burst. This problem which is modeled as a point source in a two-dimensional cylindrical (r,z) geometry with the air ground interface included, is of particular interest in the areas of nuclear weapons effects and radiation physics.

Presently the most widely used computational methods for solving the (air-over-ground) problem are Monte Carlo and discrete ordinates. However, these methods have severe limitations and computational problems. My research plan was to formulate and evaluate a solution technique which did not have these disadvantages. A finite element solution method which is based on a space-angle synthesis flux expansion of bicubic splines and spherical harmonics was chosen. The merits of this solution technique were examined and a computer algorithm for the numerical solution of this problem was developed.

I wish to acknowledge and express my appreciation for the assistance and encouragement which I have received

from the staff and students of the Air Force Institute of Technology. Special thanks are due to my advisor, Captain David D. Hardin, without whose direction, encouragement and many hours of discussion and counselling this thesis would not have been possible. I am also grateful for the support, advice and encouragement that was provided by Dr. J. Jones of the Air Force Institute of Technology Mathematics Department.

Finally, I wish to express my appreciation to my wife and daughter for their understanding, patience and constant support throughout this project. To my wife, Cynthia, I must also express a special thanks for her effort in typing this thesis.

Eze E. Wills

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Abstract

A finite element space-angle synthesis solution of the steady state anisotropic Boltzmann (transport) equation in a two-dimensional cylindrical geometry has been developed. Starting from a variational principle the Bubnov-Galerkin solution method was applied to the second order even parity form of the Boltzmann equation. A trial function flux expansion in bicubic splines and spherical (surface) harmonics was used. A first scatter (collision) source and an exponentially varying atmosphere was also incorporated into this development.

Finite element space-angle synthesis (FESAS) was developed as an alternate solution approach and an improvement in comparison to the methods of Monte Carlo and discrete ordinates. FESAS does not have the inherent characteristics which have produced the ray effect problem in discrete ordinates. Also, FESAS may result in lower computational costs than those of Monte Carlo and discrete ordinates.

The second order even parity form of the Boltzmann equation was derived and shown to be symmetric, positive definite and self-adjoint. The equivalence of a variational minimization principle and the Bubnov-Galerkin method of weighted residuals was established. The finite element space angle synthesis system of equations was

expanded and a numerical computer solution approach was implemented. A computer program was written to solve for the trial function expansion (mixing) coefficients, and also to compute the particle flux.

THE APPLICATION OF FINITE ELEMENTS AND SPACE-ANGLE SYNTHESIS TO THE ANISOTROPIC STEADY STATE BOLTZMANN (TRANSPORT) EQUATION

I Introduction

Background

The Air-Over-Ground Problem. The transport of neutrons, gamma rays and high-energy x-rays, away from a low altitude nuclear explosion (air-burst), is of special interest in assessing the vulnerability and survivability of military weapon systems and in making radiation exposure and dose predictions. This neutral particle transport problem increases in complexity because of the exponentially varying air density and the air-ground interface. A description of neutral particle transport and, therefore, the air-over-ground problem is given by the Boltzmann transport equation.

Numerical solutions to this problem already exist. The main solution techniques are Monte Carlo and discrete ordinates. However, discrete ordinates and Monte Carlo have severe difficulties and disadvantages. To perform an accurate Monte Carlo calculation requires the use of hours of costly computer time. Discrete ordinates uses less computer execution time than Monte Carlo, however, it is subject to a computational difficulty called ray effects (Ref 1:357).

Ray Effects and Discrete Ordinates. Ray effects are a result of the angular discretization of the particle flux in the discrete ordinate method. It is not a numerical problem, but originates in the derivation of the discrete ordinate S_n equations. In a physical sense these equations only allow source particles to travel in specific directions. However, in most practical problems these particles move in all directions. An in-depth analysis of the S_n equations and the nature and reasons for ray effects can be found elsewhere (Ref 1:357).

Ray effects produce non-physical distortions of the angular flux in regions where there are strong absorbers, localized sources, or high energy streaming particles (Ref 2:255-268). These distortions in the numerical formulation of the discrete ordinate method produce solutions which are inaccurate. The degree of these inaccuracies is dependent upon the specific problem and the nature of the absorbing media and sources. In the air-over-ground problem this effect will be significant because it is essentially a streaming particle problem with localized first scatter sources.

A considerable amount of work has already been done in an attempt to eliminate ray effects from the S_n equations and the discrete ordinate method. Ray effects can be mitigated by the use of a fine angular mesh in the finite differencing scheme of the S_n equations. However, this approach increases the computational time and the already

high computer costs. Other approaches involve a spherical harmonic-like formulation (Ref 2:255-268), piecewise bilinear finite element approximations (Ref 3:205-217), and space-angle synthesis with specially tailored trial functions (Ref 4:322-343).

Problem, Scope and Solution Approach

The purpose of this research project was to develop a finite element solution to the air-over-ground problem by using a space-angle synthesis of bicubic splines in space and spherical (surface) harmonics in angle. Specifically, a solution of the monoenergetic Boltzmann equation in the context of the air-over-ground problem was sought. Working from a variational principle and using a judicious choice of trial functions the problem of ray effects may be eliminated (Ref 3:214). Also, this judicious trial function choice, and a Bubnov-Galerkin solution method may be more efficient and less costly than Monte Carlo or discrete ordinates.

The steady state solution of the Boltzmann equation with first scatter sources, anisotropic scattering and an exponentially changing atmosphere is desired. The problem is formulated from a variational principle and in a two-dimensional cylindrical (r,z) spatial geometry with the air-over-ground interface included. Fluence values as a function of two spatial (r,z) and two angular (μ,χ) variables are sought. This is a four dimensional problem. Finally, a numerical solution algorithm and the computer implementation of this problem is required.

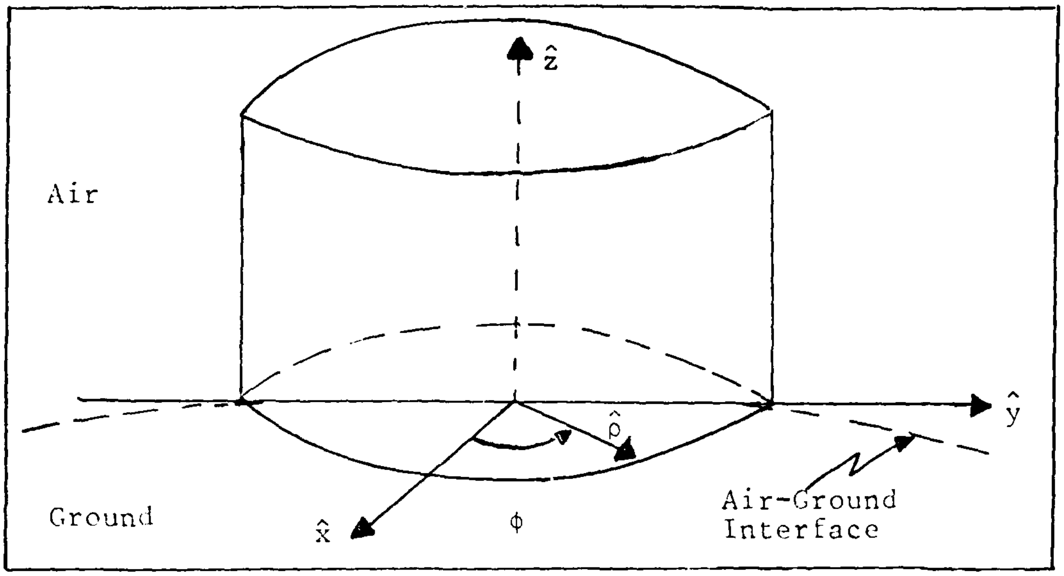

Figure 1. Cylindrical (ρ,z,ϕ) Problem Geometry

Assumptions

There are two basic assumptions which are made in the formulation of this problem. A time-independent (steady state) solution and axial symmetry is assumed. Because of the exponentially changing air density the air-over-ground problem is four dimensional with a spatially dependent (r,z) solution. An assumption of axial symmetry is made possible by ignoring the curvature of the earth. Within the problem domain of most practical problems the curvature of the earth is small and can therefore be ignored. Figure 1 shows the spatial cylindrical problem geometry.

The flux from an air burst is non-zero for a fraction of a second (microseconds). Therefore, particle fluence (number/area) and not flux is the more useful quantity. A steady state formulation of the air-over-ground problem is obtained by integrating the time dependence out of the

Boltzmann equation. This integration which is carried out over time limits when the flux is zero produces a time integrated or fluence equation.

Development

In the next chapter of this report the problem equations are presented. A finite element formulation of the air-over-ground problem is developed in Chapter III. The Bubnov-Galerkin method of weighted residuals is incorporated into this development. In Chapter IV a space-angle synthesis of bicubic splines and spherical harmonics is performed. An interpolation of the source terms is also outlined in Chapter IV. A computer implementation of the problem solution is examined in Chapter V. Finally, conclusions and recommendations are presented in Chapter VI.

II The Problem Equation

The application of finite elements and a variational principle to the air-over-ground problem and the mono-energetic steady state Boltzmann equation is not a new concept (Ref 5). As in the work by Wheaton (Ref 5) only the monoenergetic problem will be considered. It is assumed that energy dependence can be easily incorporated into this treatment by the use of standard multigroup methods. The air-over-ground problem which is in effect the steady state transport of neutral particles can be described by the Boltzmann (transport) equation and appropriate boundary conditions as follows:

$$\hat{\Omega}\cdot\nabla\phi(\hat{r},\hat{\Omega}) + \sigma_t(\hat{r})\phi(\hat{r},\hat{\Omega}) = \int_{4\pi} \sigma^s(r,\hat{\Omega}\cdot\hat{\Omega}')\phi(r,\Omega')d\Omega' + S(\hat{r},\hat{\Omega}) \qquad (1)$$

This is the one speed monoenergetic Boltzmann equation in general geometry where

$\hat{r}$ = the spatial position vector,

$\hat{\Omega}$ = a unit direction or velocity vector,

∇ = gradient operator,

ϕ = angular particle fluence in particles/unit area/steradian,

$\sigma_t(\hat{r})$ = total macroscopic interaction cross section at spatial position $\hat{r}$,

$\sigma^s(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')$ = macroscopic scattering cross section. The probability of a particle at position $\hat{r}$ and direction $\hat{\Omega}'$ scattering into direction $\hat{\Omega}$. It is a function of the scattering angle $\hat{\Omega}\cdot\hat{\Omega}'$ and not a function of the individual directions (isotropic media),

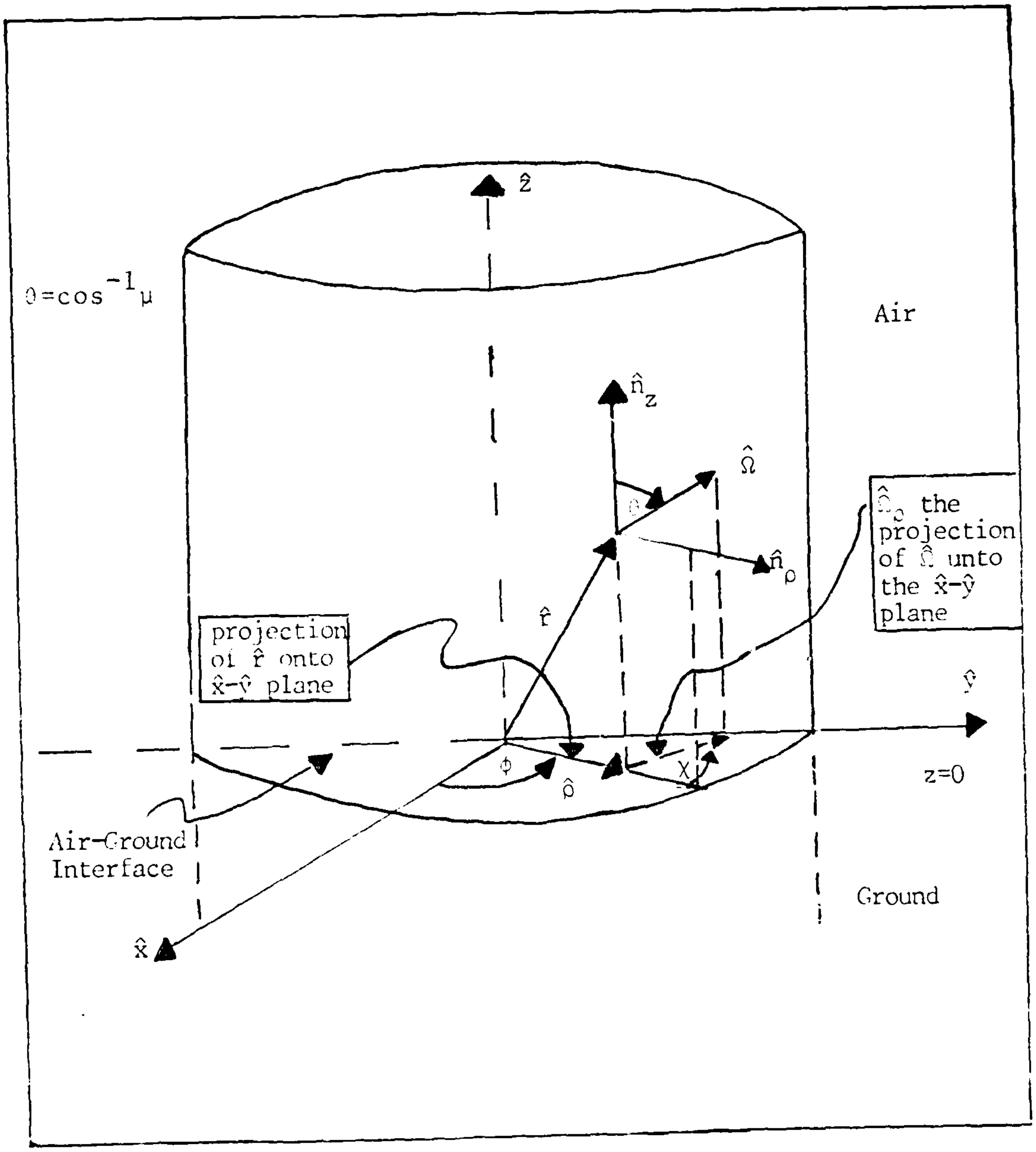

Figure 2. Problem Geometry and Coordinate System.

$S(r,\ )$ = Source density in particles/unit volume. The integration is carried out over all directions (4π steradians).

The air-over-ground problem will be formulated in cylindrical (r,z,) geometry. The coordinate system and directional angles of this system are shown in Figure 2

(Ref 6:57). μ is the cosine of the angle formed by the z-axis and the particle velocity vector $\hat{\Omega}$. χ is the angle between the planes formed by the $\hat{r}$ vector and the z-axis and that of the $\hat{\Omega}$ vector and z-axis.

The scattering properties of air show a directional dependence which is highly peaked in the forward direction especially at the high particle energies that exist in the air-over-ground problem. Because of this the exterior boundary condition for this problem will be approximated by a vacuum boundary condition:

$$\phi(\hat{r}_s, \hat{\Omega}) = 0 \text{ for } \hat{r}_s \text{ on the boundary of the problem domain and } \hat{\Omega}\cdot\hat{n} < 0 \qquad (2)$$

where $\hat{n}$ is the outward unit normal to the boundary surface. In physical terms this is a non-reentrant boundary condition. No particles are allowed to reenter the region once they leave it.

In two-dimensional cylindrical (r,z) geometry there is symmetry in the angle χ. This symmetry can be written as

$$\phi(\hat{r}, \hat{\Omega}_1) = \phi(\hat{r}, \hat{\Omega}_2) \text{ for } \hat{\Omega}_{p2} = \hat{\Omega}_{p1} - 2(\hat{n}\cdot\hat{\Omega}_{p1})\hat{n} \qquad (3a)$$

or as

$$\phi(\hat{r}, \mu, \chi) = \phi(\hat{r}, \mu, -\chi) \qquad (3b)$$

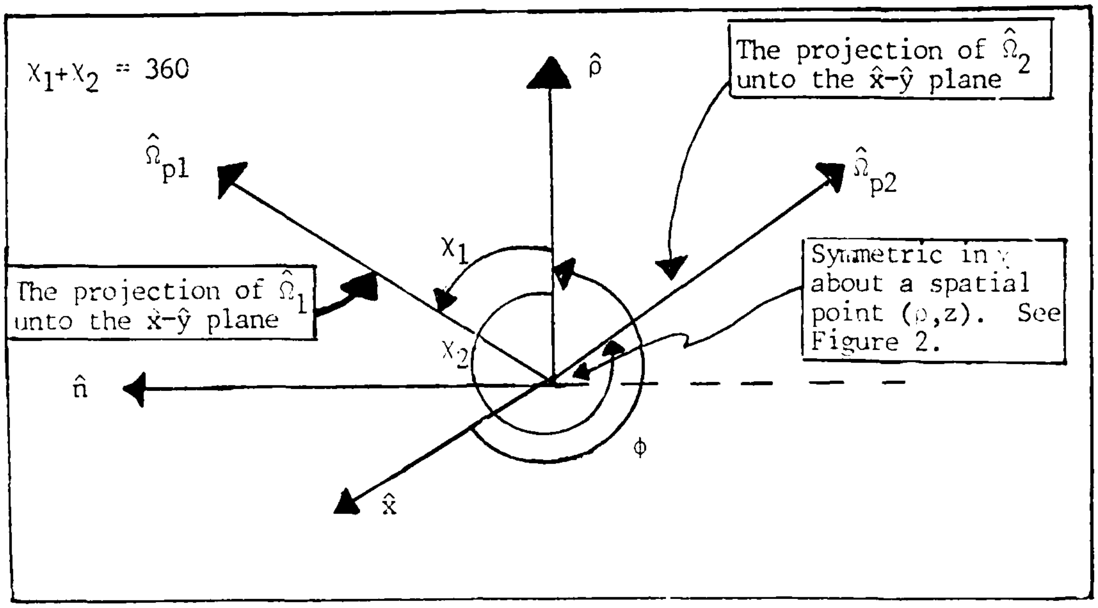

Figure 3. A Schematic of the Angular Symmetry.

This symmetry in χ is shown in Figure 3, where the vectors $\hat{n}$ and $\hat{\rho}$ are perpendicular.

Note that because of the exponentially varying air density (in the z direction), only azimuthal symmetry in the angle χ is assured. There is no symmetry in $\mu(\cos \Theta)$ and therefore $\psi(\hat{r},\hat{\Omega})$ will not be equal to $\psi(\hat{r},-\hat{\Omega})$. The symmetry condition, Eqs (3a) and (3b), implies that

$$\psi(\hat{r},\mu,\chi) = \text{even function in } \chi \tag{3c}$$

At the air ground interface $\psi(\hat{r},\hat{\Omega})$ is continuous except at $\mu = 0$ (Ref 6:160), i.e.

$$\psi_{air}(r,\Omega) = \psi_{ground}(r,\Omega) \text{ at } z = 0 \text{ and } \mu \neq 0 \tag{4}$$

However the derivatives of $\psi(\hat{r},\hat{\Omega})$ are not continuous.

The problem geometry and coordinate systems as shown in Figure 2 implies that when ρ is equal to zero the angle χ must also assume a value of zero. Therefore, along the z axis (ρ=0) the angle χ does not vary between 0 and 2π. This means that there is no χ variation in $\phi(\hat{r},\hat{\Omega})$ at ρ=0 and that

$$\frac{\partial}{\partial \chi}\phi(\hat{r},\hat{\Omega}) = 0 \text{ for } \hat{\rho}=0 \tag{5}$$

III The Finite Element Method

The finite element method is a mathematical and numerical technique for approximating the solution to a large class of problems. Initially it was developed and used to solve problems in stress analysis (Ref 7:9). Later, as the mathematical foundation of the method was established it gained widespread acceptance and use in solving a larger class of problems.

Finite elements are an extension of the Rayleigh-Ritz technique of first recasting the problem in an equivalent variational form and then seeking a solution on the basis of an energy minimization principle (Ref 8:1). In the Rayleigh-Ritz method a solution in the form of a linearly independent set of trial functions is assumed. These trial functions must satisfy the essential boundary conditions. The approximate or "best" solution to the problem is the linear combination of these trial functions which maximizes (or minimizes) the variational principle (functional). If this linear combination of functions is not an extremum (maximum or minimum) of the functional, then the class (or space) of trial functions is expanded by the addition of more functions. This expansion of the trial function space is continued until a linear combination of functions which is an extremum of the functional is obtained.

The finite element solution technique is similar to that of Rayleigh-Ritz. The only difference lies in the

choice of trial functions. In finite elements the problem domain is divided into smaller regions (grids) or elements. Each trial function is usually associated with only a few elements. Unlike Rayleigh-Ritz, finite elements uses trial functions which are zero over parts of the solution domain (a local basis). Also, the trial space (number of trial functions) is expanded by using more elements (mesh points) and not by the addition of a new class of functions. Because of these differences the finite element method is more adaptable towards a numerical (computer) solution than Rayleigh-Ritz.

There are two basic approaches to the finite element formulation of a problem. One approach is to find the extremum of the functional which originates from a variational principle and the calculus of variations (Rayleigh-Ritz with a local basis). The other is by the method of weighted residuals. The method of weighted residuals does not include the use of a variational principle or the calculus of variations. In some problems a variational principle has not been developed or may not exist, and therefore, the Rayleigh-Ritz approach cannot be used. However, in such cases, the method of weighted residuals can be used to solve the problem. Therefore, the method of weighted residuals can be extended to a wider class of problems than Rayleigh-Ritz.

The method of weighted residuals is another approach for developing a set of (algebraic) problem equations to which the finite element method can be applied. There are

three basic mathematical "recipes" through which the method of weighted residuals can be developed. These are the methods of least squares, collocation and Galerkin. In some problems where a variational principle (functional) exists it can be shown (Ref 9:735) that the Galerkin method of weighted residuals is equivalent to Rayleigh-Ritz. An identical set of matrix equations and therefore the same solution is achieved by either method.

In the following paragraphs a variational principle for the air-over-ground problem and the even parity form of the Boltzmann equation is examined. A weak form of the variational principle and the boundary conditions are incorporated within this development. Finally, the Galerkin method of weighted residuals is discussed and an equivalence to the variational approach for the air-over-ground problem is established.

Even and Odd Parity Second Order Forms

In order that a variational principle may be used the even and odd parity forms of the anisotropic Boltzmann equation and associated boundary conditions will be developed. The starting point of this development is Eqs (1) and (2). Following the derivation of Kaplan and Davis (Ref 10:166) and that of Wheaton (Ref 5) the *mono-energetic* steady state transport equation can be written in terms of the $-\hat{\Omega}$ vector by changing $\hat{\Omega}$ to $-\hat{\Omega}$ in Eq (1). This gives

$$-\hat{\Omega}\cdot\nabla\phi(\hat{r},-\hat{\Omega}) + \sigma_t(\hat{r})\phi(\hat{r},-\hat{\Omega}) = \int \sigma^s(\hat{r},-\hat{\Omega}\cdot\hat{\Omega}')\phi(\hat{r},\hat{\Omega}')d\hat{\Omega}' + Q(\hat{r},-\hat{\Omega}) \qquad (6)$$

The even and odd parity terms will now be defined as

$$\Psi(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\{\phi(\hat{r},\hat{\Omega}) + \phi(\hat{r},-\hat{\Omega})\} \tag{7}$$

$$\chi(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\{\phi(\hat{r},\hat{\Omega}) - \phi(\hat{r},-\hat{\Omega})\} \tag{8}$$

$$S^{g}(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\{S(\hat{r},\hat{\Omega}) + S(\hat{r},-\hat{\Omega})\} \tag{9}$$

$$S^{u}(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\{S(\hat{r},\hat{\Omega}) - S(\hat{r},-\hat{\Omega})\} \tag{10}$$

$$\sigma^{g}(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') = \tfrac{1}{2}\{\sigma^{s}(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') + \sigma^{s}(\hat{r},-\hat{\Omega}\cdot\hat{\Omega}')\} \tag{11}$$

$$\sigma^{u}(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') = \tfrac{1}{2}\{\sigma^{s}(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') - \sigma^{s}(\hat{r},-\hat{\Omega}\cdot\hat{\Omega}')\} \tag{12}$$

where

$\Psi(\hat{r},\hat{\Omega})$ = even parity fluence

$\chi(\hat{r},\hat{\Omega})$ = odd parity fluence

$S^{g}(\hat{r},\hat{\Omega})$ = even parity source

$S^{u}(\hat{r},\hat{\Omega})$ = odd parity source

$\sigma^{g}(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')$ = even parity scattering cross-section

$\sigma^{u}(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')$ = odd parity scattering cross-section

Adding Eqs (1) and (6), then dividing throughout by two and using the above definitions gives

$$\hat{\Omega}\cdot\nabla\chi(\hat{r},\hat{\Omega}) + \sigma_{t}(\hat{r})\Psi(\hat{r},\hat{\Omega}) = \int_{4\pi}\sigma^{g}(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\phi(\hat{r},\hat{\Omega}')d\Omega' + S^{g}(\hat{r},\hat{\Omega}) \tag{13}$$

Using the derivation of Wheaton (Ref 5:8), which is also reproduced in Appendix A, the scattering kernel term in (13) can be written as

$$\int_{4\pi}\sigma^{g}(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\phi(\hat{r},\hat{\Omega}')d\Omega' = \int_{4\pi}\sigma^{g}(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\Psi(\hat{r},\hat{\Omega}')d\Omega' \tag{14}$$

where the even properties of the even parity scattering cross-section and the even parity fluence have been used in the derivation of Eq (14). Eq (13) now becomes

$$\hat{\Omega}\cdot\nabla\chi(\hat{r},\hat{\Omega}) + \sigma_t(\hat{r})\Psi(\hat{r},\hat{\Omega}) = \int_{4\pi}\sigma^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\Psi(\hat{r},\hat{\Omega}')d\hat{\Omega}' + S^g(\hat{r}.\hat{\Omega}) \tag{15}$$

Similarly, by substracting Eqs (1) and (6) and rearranging the scattering kernel (See Appendix A) gives

$$\hat{\Omega}\cdot\nabla\Psi(\hat{r},\hat{\Omega}) + \sigma_t(\hat{r})\chi(\hat{r},\hat{\Omega}) = \int_{4\pi}\sigma^u(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\chi(\hat{r},\hat{\Omega}')d\hat{\Omega}' + S^u(\hat{r},\hat{\Omega}) \tag{16}$$

Eqs (15) and (16) are referred to by Kaplan and Davis (Ref 10) as canonical forms. The natural boundary condition Eq (2) can also be rewritten as

$$\Psi(\hat{r}_s,\hat{\Omega}) + \chi(\hat{r}_s,\hat{\Omega}) = 0 \text{ for } \hat{\Omega}\cdot\hat{n} < 0 \tag{17}$$

and

$$\Psi(\hat{r}_s,\hat{\Omega}) - \chi(\hat{r}_s,\hat{\Omega}) = 0 \text{ for } \hat{\Omega}\cdot\hat{n} > 0 \tag{18}$$

The symmetric conditions Eqs (3a) and (3c) now become

$$\Psi(\hat{r},\hat{\Omega}_1) + \chi(\hat{r},\hat{\Omega}_1) = \Psi(\hat{r},\hat{\Omega}_2) + \chi(\hat{r},\hat{\Omega}_2) \quad \text{for } \hat{\Omega}_{p2} = \hat{\Omega}_{p1} - 2(\hat{\Omega}_{p1}\cdot\hat{n})\hat{n} \tag{19}$$

where $\Psi(r,\Omega)$ and $\chi(r,\Omega)$ must be even functions in the azimuthal angle ϕ (see Fig. 3). Therefore it follows that for $\hat{\Omega}_{p2} = \hat{\Omega}_{p1} - 2(\hat{\Omega}_{p1}\cdot\hat{n})\hat{n}$

$$\Psi(\hat{r},\hat{\Omega}_1) = \Psi(\hat{r},\hat{\Omega}_2) \tag{20}$$

and

$$\chi(\hat{r},\hat{\Omega}_1) = \chi(\hat{r},\hat{\Omega}_2) \tag{21}$$

Also $\chi(\hat{r},\hat{\Omega})$ and $\Psi(\hat{r},\hat{\Omega})$ are continuous at the air ground interface (when $\mu \neq 0$) but their derivatives are discontinuous.

A further simplification is now introduced into this development by defining the even and odd operators, G^g and G^u as

$$G^g(\hat{r})f(\hat{r},\hat{\Omega}) = \sigma_t(\hat{r})f(\hat{r},\hat{\Omega}) - \int_{4\pi}\sigma^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')f(\hat{r},\hat{\Omega}')d\hat{\Omega}' \tag{22}$$

$$G^u(\hat{r})f(\hat{r},\hat{\Omega}) = \sigma_t(\hat{r})f(\hat{r},\hat{\Omega}) - \int_{4\pi}\sigma^u(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')f(\hat{r},\hat{\Omega}')d\hat{\Omega}' \tag{23}$$

where the scattering cross sections can be expanded in spherical (surface) harmonics (see Appendix A) to give

$$G^g(\hat{r})f(\hat{r},\hat{\Omega}) = \sigma_t(\hat{r})f(\hat{r},\hat{\Omega})$$
$$- \Sigma_\ell\Sigma_m\sigma_\ell^g(\hat{r})Y_{\ell m}(\hat{\Omega})\int_{4\pi}Y_{\ell m}^*(\hat{\Omega}')f(\hat{r},\hat{\Omega}')d\hat{\Omega}' \tag{24}$$

where the even parity Legendre expansion cross-section σ_ℓ^g is defined as

$$\sigma_\ell^g(\hat{r}) = \begin{cases} \sigma_\ell^s(\hat{r}) & \text{for } \ell \text{ even} \\ 0 & \text{for } \ell \text{ odd} \end{cases} \tag{25}$$

and

$\sigma_\ell^s(\hat{r})$ = Legendre expansion scattering cross-section coefficients (Ref 5:29)

The derivation of $\sigma_\ell^g(\hat{r}) = \sigma_\ell^s(r)_{\text{even}}$ can be found in Appendix A.

The odd parity scattering cross section can also be expanded to give

$$G^u(\hat{r})f(\hat{r},\hat{\Omega}) = \sigma_t(\hat{r})f(\hat{r},\hat{\Omega}) - \sum_\ell \sum_m \sigma_\ell^u(\hat{r})Y_{\ell m}(\hat{\Omega})\int_{4\pi} Y^*_{\ell m}(\hat{\Omega}')f(\hat{r},\hat{\Omega}')d\hat{\Omega}' \quad (26)$$

where only odd expansions in ℓ are used or σ_ℓ^u is defined as

$$\sigma_\ell^u(\hat{r}) = \begin{cases} \sigma_\ell^s(r) & \text{for } \ell \text{ odd} \\ 0 & \text{for } \ell \text{ even} \end{cases} \quad (27)$$

The G^g and G^u operators are self adjoint positive definite (Ref 10:174). Inserting these operators into Eqs (15) and (16) they become

$$G^g(\hat{r})\Psi(\hat{r},\hat{\Omega}) = S^g(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla\chi(\hat{r},\hat{\Omega}) \quad (28)$$

and

$$G^u(\hat{r})\chi(\hat{r},\hat{\Omega}) = S^u(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla\Psi(\hat{r},\hat{\Omega}) \quad (29)$$

Solving for $\Psi(\hat{r},\hat{\Omega})$ and $\chi(\hat{r},\hat{\Omega})$ from Eqs (28) and (29) produces

$$\Psi(\hat{r},\hat{\Omega}) = \left[G^g(\hat{r})\right]^{-1}\left\{S^g(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla\chi(\hat{r},\hat{\Omega})\right\} \quad (30)$$

$$\chi(\hat{r},\hat{\Omega}) = \left[G^u(\hat{r})\right]^{-1}\left\{S^u(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla\Psi(\hat{r},\hat{\Omega})\right\} \quad (31)$$

where using the notation of Kaplan and Davis

$$K^u(\hat{r}) = \{G^u(\hat{r})\}^{-1} = \text{inverse of the operator } G^u(\hat{r}) \quad (32)$$

$$K^g(\hat{r}) = \{G^g(\hat{r})\}^{-1} = \text{inverse of the operator } G^g(\hat{r}) \quad (33)$$

A detailed mathematical derivation of these inverse operators is presented in Appendix A. They are defined as (Ref 11:481)

$$K^g(\hat{r}) = \sigma_t^{-1}(\hat{r})\Big[1$$
$$+ \Sigma_\ell \Sigma_m \{\sigma_\ell^g(\hat{r})/(\sigma_t(\hat{r})-\sigma_\ell^g(\hat{r}))\} Y_{\ell m}(\hat{\Omega}) \int_{4\pi} Y^*_{\ell m}(\hat{\Omega}')d\hat{\Omega}'\Big] \quad (34)$$

where $\sigma_\ell^g(\hat{r})$ is defined by Eq (25).

$$K^u(\hat{r}) = \sigma_t^{-1}(r)\Big[1$$
$$+ \Sigma_\ell \Sigma_m \{\sigma_\ell^u(r)/(\sigma_t(\hat{r})-\sigma_\ell^u(\hat{r}))\} Y_{\ell m}(\hat{\Omega}) \int_{4\pi} Y^*_{\ell m}(\hat{\Omega}')d\hat{\Omega}'\Big] \quad (35)$$

Both K^u and K^g must be self adjoint positive definite since they are the inverses of G^u and G^g which are both positive definite and self adjoint.

The functions $Y_{\ell m}(\hat{\Omega})$ and $Y^*_{\ell m}(\hat{\Omega})$ are the well known normalized spherical (surface) harmonics (Ref 6:609) which are defined as

$$Y_{\ell m}(\hat{\Omega}) = Y_{\ell m}(\mu,\chi) = \sqrt{\frac{2\ell+1}{4\pi} \cdot \frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^m(\mu)e^{im\chi} \quad (36)$$

and $Y^*_{\ell m}(\hat{\Omega})$ being the complex conjugate of $Y_{\ell m}(\hat{\Omega})$ is defined as

$$Y^*_{\ell m}(\hat{\Omega}) = Y^*_{\ell m}(\mu,\chi) = \sqrt{\frac{2\ell+1}{4\pi} \cdot \frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^m(\mu)e^{-im\chi} \quad (37)$$

where $\mu = \cos\theta$ and $P_\ell^m(\mu)$ is the associated Legendre functions.

Eqs (30 and (31) can now be written as

$$\Psi(\hat{r},\hat{\Omega}) = K^g(\hat{r})\{S^g(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla\chi(\hat{r},\hat{\Omega})\} \quad (38)$$

and

$$\chi(\hat{r},\hat{\Omega}) = K^u(\hat{r})\{S^u(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla\Psi(\hat{r},\hat{\Omega})\} \tag{39}$$

Substituting Eq (39) into Eq (28) produces the second order even parity form of the Boltzmann equation

$$-\hat{\Omega}\cdot\nabla K^u(\hat{r})\hat{\Omega}\cdot\nabla\Psi(\hat{r},\hat{\Omega}) + G^g(\hat{r})\Psi(\hat{r},\hat{\Omega}) = S^g(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla K^u(\hat{r})S^u(\hat{r},\hat{\Omega}) \tag{40}$$

and inserting Eq (39) into Eqs (17) and (18) gives the appropriate surface boundary conditions for Eq (40) as

$$\Psi(\hat{r}_s,\hat{\Omega}) + K^u(\hat{r}_s)\{S^u(\hat{r}_s,\hat{\Omega}) - \hat{\Omega}\cdot\nabla\Psi(\hat{r}_s,\hat{\Omega})\} = 0 \text{ for } \hat{\Omega}\cdot\hat{n} < 0 \tag{41}$$

and

$$\Psi(\hat{r}_s,\hat{\Omega}) - K^u(\hat{r}_s)\{S^u(\hat{r}_s,\hat{\Omega}) - \hat{\Omega}\cdot\nabla\Psi(\hat{r}_s,\hat{\Omega})\} = 0 \text{ for } \hat{\Omega}\cdot\hat{n} > 0 \tag{42}$$

Eqs (38) and (39) give the second order odd parity form of the Boltzmann equation which is

$$-\hat{\Omega}\cdot\nabla K^g(\hat{r})\hat{\Omega}\cdot\nabla\chi(\hat{r},\hat{\Omega}) + G^u(\hat{r})\chi(\hat{r},\hat{\Omega}) = S^u(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla K^g(\hat{r})S^g(\hat{r},\hat{\Omega}) \tag{43}$$

Inserting Eq (38) into Eqs (17) and (18) the surface boundary conditions for Eq (43) are

$$\chi(\hat{r}_s,\hat{\Omega}) + K^g(\hat{r})\{S^g(\hat{r}_s,\hat{\Omega}) - \hat{\Omega}\cdot\nabla\chi(\hat{r}_s,\hat{\Omega})\} = 0 \text{ for } \hat{\Omega}\cdot\hat{n} < 0 \tag{44}$$

and

$$\chi(\hat{r}_s,\hat{\Omega}) - K^g(\hat{r})\{S^g(\hat{r}_s,\hat{\Omega}) - \hat{\Omega}\cdot\nabla\chi(\hat{r}_s,\hat{\Omega})\} = 0 \text{ for } \hat{\Omega}\cdot n > 0 \tag{45}$$

The Variational Principle

Variational principles for the monoenergetic transport equation have been found. These principles are related by a series of transformations (Ref 10:166). The functional whose Euler equations are the even and odd parity second order Boltzmann equations will be used in this work. Primarily the even parity component will be used because it is always positive, self-adjoint and can be integrated to give the scalar flux or fluence (Ref 12:148). The odd-parity flux which can be negative integrates (over all directions) into the net current (Ref 13:12). Another "nice" feature of this even and odd parity formulation is that it produces a solution matrix which is positive definite and symmetric.

Defining the inner product of two functions as

$$\langle f,g\rangle = \int_{4\pi} f^{*}(\hat{\Omega})\,g(\hat{\Omega})\,d\hat{\Omega} \tag{46}$$

where $*$ means the complex conjugate, the functional which corresponds to Eqs (40) (41) and (42) is given as (Ref 10:169)

$$F(u) = \int_R \{\langle\hat{\Omega}\cdot\nabla u, K^u(\hat{\Omega}\cdot\nabla u)\rangle + \langle u, C^g u\rangle - 2\langle\hat{\Omega}\cdot\nabla u, K^u S^u\rangle - 2\langle u, S^g\rangle\}\,d\vec{r} - \oint_S \{\int_{4\pi} |\hat{\Omega}\cdot\hat{n}|\,u^2\,d\hat{\Omega}\}\,d\hat{S} \tag{47}$$

where $\oint_S$ represents a surface integral.

It can be shown Ref (10:169) that the Euler equation (stationary point) of this functional is indeed the even parity second order form of the Boltzmann equation and that Eqs (41) and (42) are the natural boundary conditions. A similar functional for the odd parity equation has also been found.

In Appendix B the stationary point of Eq (47) is shown to be a minimum and the weak or Galerkin form is obtained. This weak form is

$$\int_R \{ (\hat{\Omega}\cdot\nabla\eta, K^u(\hat{\Omega}\cdot\nabla\Psi)> + <\eta, G^g\Psi> \} d\hat{r} + \oint_S \int_{4\pi} |\hat{\Omega}\cdot\hat{n}| \eta\Psi d\hat{\Omega} d\hat{s}$$
$$= \int_R \{ <\hat{\Omega}\cdot\nabla\eta, K^u S^u> + <\eta, S^g> \} d\hat{r} \qquad (48)$$

where

η = test or weight function

and

Ψ = trial function

The natural boundary conditions Eqs (41) and (42) are incorporated into the weak form of equation (48). However, the boundary condition at the ground interface is an essential condition. A solution to the air-over-ground problem can be obtained from a solution to Eq (48) and this essential boundary condition.

The Galerkin or weak form of Eq (48) produces a solution matrix which is positive definite and symmetric. It is symmetric because the test and trial functions are the same in the Galerkin solution method. The matrix is positive definite because K^u and G^g are positive definite and it is obvious that for the Galerkin solution the term $<\hat{\Omega}\cdot\nabla\eta, K^u(\hat{\Omega}\cdot\nabla\Psi)>$ is also positive definite.

The Method of Weighted Residuals

The method of weighted residuals is a straightforward and simple prescription for solving a wide class of problems.

Unlike Rayleigh-Ritz it does not depend on a variational principle or the calculus of variations. However, in solving certain types of problems the use of a variational principle or the Galerkin method of weighted residuals is equivalent and they produce solutions which are identical. For the air-over-ground problem and the second order even parity form of the Boltzmann equation it will be shown that the Galerkin method and the weak form, which is given by Eq (48), are equivalent formulations of the same problem.

In the method of weighted residuals an approximate solution which is a linear combination of trial functions is assumed to exist. These trial functions are required to satisfy the necessary boundary and continuity conditions. The approximate solution, when inserted into the problem equation, is then required to be an exact solution of the problem with respect to several weight functions (Ref 7:106). The choice of weight functions determines whether the method of weighted residuals is one of collocation, least squares or Galerkin. In the Galerkin method the weight functions are chosen to be the same as the trial functions.

Applying the Galerkin method of weighted residuals to the second order form of the Boltzmann equation is equivalent to using a variational principle. In Appendix C the weak form, Eq (48), is derived from a Galerkin formulation of this problem. The natural boundary condition is incorporated into this development and an equation identical to Eq (48)

is produced. Therefore, solutions to the second order form of the Boltzmann equation, by using a variational principle or the Galerkin method of weighted residuals are equivalent. This equivalency exists because the second order even parity operator of Eq (40) is positive definite and self-adjoint.

IV Space-Angle Synthesis of the Even-Parity Anisotropic Boltzmann Equation

A space angle synthesis solution approach has already been applied to the air-over-ground problem. Roberds and Bridgman used "specially tailored" angular trial functions to solve the two dimensional steady state anisotropic Boltzmann equation Ref (4:332). Space angle synthesis was applied directly to Eq (1), and not to the second order form of the Boltzmann equation. Miller et al. (Ref 13:12) have applied phase-space finite elements directly to the isotropic second order Boltzmann equation in x - y geometry. Wheaton (Ref 5) has applied phase-space finite elements to the air-over-ground problem. However a space angle synthesis finite element approach using a flux expansion in bicubic splines and spherical harmonics has not been done.

Because of the complexity of the air-over-ground problem a space-angle synthesis finite element approach seems to be justified. This solution technique might have several advantages, some of which are:

1. The elimination of ray effects;
2. The numerical advantages of finite elements in combination with a space-angle synthesis approach, may be able to better handle the four-dimensionality of the problem;
3. Anisotropic scattering can be easily handled by a "wise and convenient" choice of angular trial functions;

4. The computational effort might be reduced, without a loss in accuracy. It is expected that bicubic splines will not require a fine spatial problem grid (mesh size); and
5. The boundary conditions and a first scatter source formulation can be easily handled.

The finite element space-angle synthesis technique is merely a spatial and angular expansion of the even parity flux by a tensor product of polynomial functions and spherical harmonics. In this work a tensor product of bicubic polynomial splines is used. This expansion is the trial solution which will be used in the finite element method. The piecewise bicubic spline expansion becomes a local basis in the spatial (ρ,z) variable. However, the spherical (surface) harmonics which are defined throughout the angular problem domain form a global basis. Therefore, this trial function expansion has a dual basis -- a local basis in space and a global basis in angle. This is the finite element space angle synthesis method.

The starting point of this development is the weak form of the second order even parity Boltzmann equation and essential boundary conditions. The air-over-ground problem is described by the weak form of Eq (48) and the symmetric condition Eq (20). An essential boundary condition, at the air ground interface, is that $\Psi(\hat{r},\hat{\Omega})$ is continuous at $z = 0$ and $\mu \neq 0$ (see Fig. _). However, the derivatives of $\Psi(\hat{r},\hat{\Omega})$ are discontinuous.

In the remainder of this section the spatial and angular trial functions will be examined. A system of coupled equations for the numerical solution of the air-over-ground problem will be developed. A first scatter (collision) source will be used in this development.

The Trial Functions

Because this is a four dimensional problem with anisotropic scattering a numerical solution technique is required. The finite element formulation of this problem lends itself directly to such a solution approach. However an application of four dimensional phase-space finite elements to Eq (48) will be very costly (computer costs) and inefficient (Ref 5:33). This is due to the added complexity of anisotropic scattering. Anisotropic scattering increases the bookkeeping and computational difficulties. A local elemental basis in angle requires that the scattering contribution to each element must be computed on an element by element basis for all space and angle elements within the problem domain. Therefore a four-dimensional phase-space finite element formulation of this problem is not a very attractive or realistic approach.

A close examination of Eq (48) shows that the problem operator is self-adjoint positive definite symmetric. This allows the use of standard matrix iterative solution techniques such as Gauss-Seidel, Jacobi or Successive over-relaxation (Ref 14:183). Therefore, a numerical method that includes a finite element solution might be feasible

if the anisotropic scattering contributions can be effectively dealt with. A space-angle synthesis finite element development with a local spline basis in space and a global spherical harmonic basis in angle appears to meet this requirement.

A phase-space finite element problem formulation which eliminated the characteristic lines of the hyperbolic discrete ordinate S_n equations has been effective in mitigating ray effects (Ref 3:205). The well known P_N and double-P_N equations of nuclear reactor physics have inherent elliptic features which eliminate ray effects. Therefore space-angle synthesis using spherical harmonics seems to represent an approach which will eliminate ray effects.

The trial function expansion which will be used in this development is

$$\Psi(z,\rho,\mu,\chi) = \sum_{iz=1}^{IZ} \sum_{ir=1}^{IR} \sum_{\ell=0}^{+L} \sum_{m=-\ell}^{+\ell} A_{\substack{iz,ir\\ \ell,m}} B_{iz}(z) \cdot B_{ir}(\rho) Y_{\ell m}(\mu,\chi) \tag{49}$$

where ρ,z is the spacial coordinate dependence in cylindrical geometry and μ,χ represents the $\hat{\Omega}$ angular variable in Fig. 2.

$\Psi(z,\rho,\mu,\chi)$ = even parity fluence at position r,z and in direction μ,χ,

$A_{\substack{iz,ir\\ \ell,m}}$ = flux expansion or mixing coefficients,

$B_{iz}(z)$ cubic polynomial spline in the z-variable (z-spline),

$B_{ir}(\rho)$ = cubic polynomial ρ-spline,

$Y_{\ell m}(\mu,\chi)$ = spherical harmonic function, Eq (51).

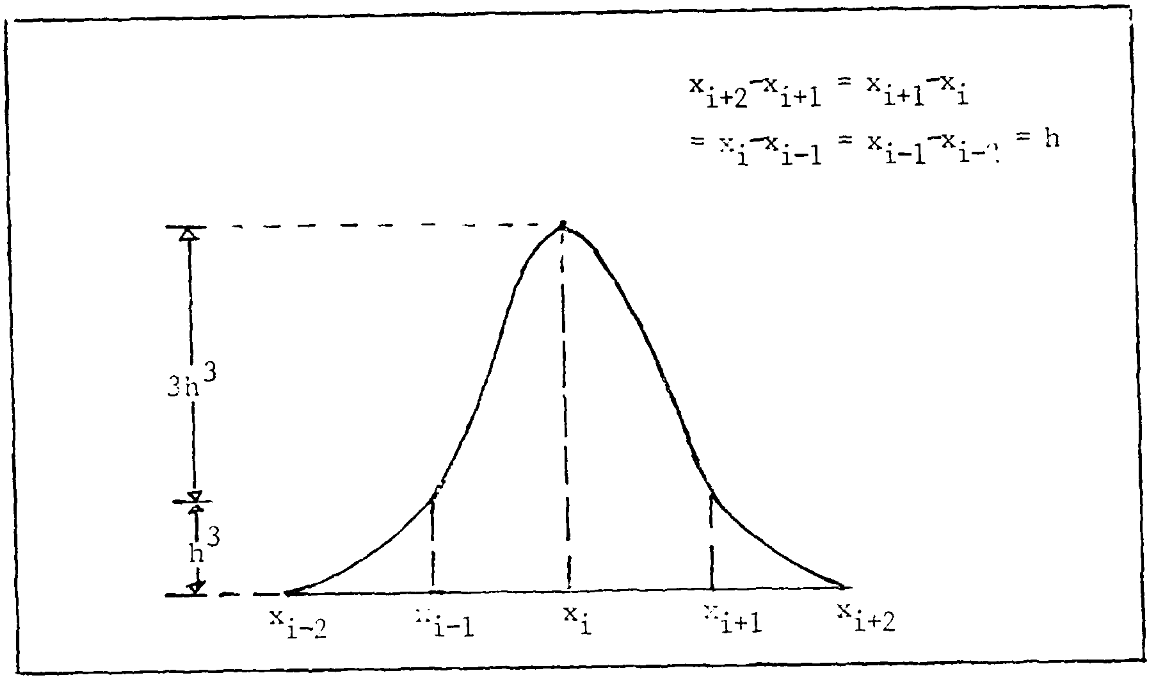

Figure 4. Cubic Spline With Evenly Spaced Nodes

iz, ir, ℓ and m are the trial function summation indices and

IZ = total number of z-splines,

IR = total number of ρ-splines,

L = degree of the spherical harmonic expansion.

The definition of a cubic polynomial splines (Ref 15:89) with evenly spaced nodes (knots) is

$$S_i(x) = \begin{cases} (x_{i+2}-x)^3, & x_{i+1} \leqslant x \leqslant x_{i+2} \\ (x_{i+2}-x)^3-4(x_{i+1}-x)^3, & x_i \leqslant x \leqslant x_{i+1} \\ (x_{i+2}-x)^3-4(x_{i+1}-x)^3+6(x_i-x)^3, & x_{i-1} \leqslant x \leqslant x_i \\ (x_{i+2}-x)^3-4(x_{i+1}-x)^3+6(x_i-x)^3-4(x_{i-1}-x)^3, & x_{i-2} \leqslant x \leqslant x_{i-1} \end{cases} \qquad (30)$$

The graph of this spline function is shown in Fig. 4. The spherical harmonic function (Ref 6:609) will be defined as

$$Y_{\ell m}(\mu,\chi) = C_{\ell m}P_{\ell m}(\mu)e^{im\chi} = C_{\ell m}P_{\ell m}(\mu)\{\cos(m\chi) + i\sin(m\chi)\} \tag{51}$$

where

$$C_{\ell m} = \sqrt{\frac{2\ell + 1}{4\pi} \cdot \frac{(\ell - m)!}{(\ell + m)!}} \tag{52}$$

The trial function expansion, Eq (49) can be made to satisfy the symmetry of Eq (20). This is a symmetric condition in χ which directly implies that the solution must also be an even function in the variable χ. Therefore, the angular trial function expansion of Eq (49) must also be even in χ. Dropping the $i\sin(m\chi)$ term from Eq (51) and substituting into Eq (49) gives

$$\Psi(z,\rho,\mu,\chi) = \sum_{iz=1}^{IZ} \sum_{ir=1}^{IR} \sum_{\ell=0}^{L} \sum_{m=0}^{\ell} A_{iz,ir,\ell,m} B_{iz}(z) \cdot B_{ir}(\rho) \cdot Q_{\ell m} \tag{53}$$

where

$$Q_{\ell m} = C_{\ell m}P_{\ell m}(\mu)\cos(m\chi) \tag{54}$$

and by using the orthonormal properties of spherical harmonics the m index begins at zero instead of $-\ell$ (see Appendix D).

The essential boundary condition at the air ground interface must also be applied to Eq (53). The fluence continuity requirements can be satisfied by this expansion in bicubic polynomial splines and spherical harmonics. Both of these functions are continuous throughout the problem domain. The cubic splines are also twice continuously

differentiable but the spatial z-derivative of the solution fluence is not continuous at the ground interface. However, the z-splines can be modified to have discontinuous derivatives at this interface (Ref 16). A Double-P_N or Yvon's method (Ref 6:163) can also be used to accomodate the fluence discontinuity at $\mu = 0$. In this development the air-ground interface will not be included in the problem domain, and therefore, this interface boundary condition will not be enforced.

Since a Galerkin method is being used the test or weight functions are

$$\eta(z,\rho,\mu,\chi) = B_{jz}(z)\, B_{jr}(\rho) Q_{kn} \tag{55}$$

Substituting Eqs (55) and (53) into Eq (48) produces Eq (58) where for simplicity the ρ, z, μ, χ dependencies are omitted and

$$B_i = B_{iz}(z) B_{ir}(\rho) \tag{56}$$

and

$$B_j = B_{jz}(z) B_{jr}(\rho) \tag{57}$$

$$\sum_{iz=1}^{IZ} \sum_{ir=1}^{IR} \sum_{\ell=0}^{L} \sum_{m=0}^{\ell} A_{\substack{ij\\ \ell m}} \Big[\int_R \{ \langle \hat{\Omega}\cdot\nabla(B_j \cdot Q_{kn}), K^u(\hat{\Omega}\cdot\nabla(B_i Q_{\ell m})) \rangle + \langle B_j Q_{kn}, G^g(B_i Q_{\ell m}) \rangle \} dr + \oint_s \int_{\hat{n}\cdot\hat{\Omega}<0} |\hat{\Omega}\cdot\hat{n}| B_j Q_{kn} B_i Q_{\ell m}\, d\Omega\, ds \Big]$$
$$= \int_R \{ \langle \hat{\Omega}\cdot\nabla (B_j Q_{kn}), K^u S^u \rangle + \langle B_j Q_{kn}, S^g \rangle \} dr \tag{58}$$

This is a system of coupled algebraic equations where the unknown quantities are the $A_{ij\ell m}$ mixing coefficients. Eq (58) can also be written as

$$\underset{N\times N}{\left[\bar{K}\right]}\ \underset{N\times 1}{\left[\bar{A}\right]} = \underset{N\times 1}{\left[\bar{S}\right]} \tag{59}$$

where

$$N = IZ \cdot IR \cdot (L+1) \cdot (L+2)/2 \tag{60}$$

$\bar{K}$ = Coefficient or stiffness matrix, where each element is a summation of terms in the square brackets of Eq (58)

$\bar{A}$ = $A_{ij\ell m}$ mixing coefficient vector

$\bar{S}$ = Source vector which is the right hand side of Eq (58)

The $A_{ij\ell m}$ coefficients of Eq (53) will be obtained from a computer solution of Eq (59). These mixing coefficients can then be substituted into Eq (53) to give the even parity fluence, $\psi(z,\rho,\mu,\chi)$. In a solution of Eq (59) the elements of the K matrix and S vector must be computed. This computation involves an evaluation and summation of the individual expanded terms of Eq (58). This expansion is carried out in Appendix E.

The directional gradient operator in cylindrical geometry is defined as (Ref 6:59)

$$\hat{\Omega}\cdot\nabla\phi = \frac{\sqrt{1-\mu^2}\cos\chi}{\rho}\frac{\partial(\rho\phi)}{\partial\rho} - \frac{1}{\rho}\frac{\partial\{\phi\sqrt{1-\mu^2}\sin\chi\}}{\partial\chi} + \mu\frac{\partial\phi}{\partial z} \tag{61}$$

This is the conservative form of the directional derivative in two dimensional (ρ,z) geometry with azimuthal symmetry.

The K^u and G^g operators have been defined in Eqs (24) and (35) of Chapter III. The scalar product of the velocity and normal vectors is given in Appendix E as

$$\hat{\Omega}\cdot\hat{n} = \begin{cases} \hat{\Omega}\cdot\hat{n}_z & \text{for the horizontal outer surfaces (top or bottom) of the problem cylinder, and as} \\ \hat{\Omega}\cdot\hat{n}_\rho & \text{for the vertical surface (side) of the cylinder} \end{cases} \tag{62a}$$

where

$$\hat{\Omega}\cdot\hat{n}_z = \begin{cases} \mu & \text{on the top surface, and} \\ -\mu & \text{on the bottom surface} \end{cases} \tag{62b}$$

and

$$\hat{\Omega}\cdot\hat{n}_\rho = \sqrt{1-\mu^2}\,\cos\chi \tag{62c}$$

The normal unit vectors $\hat{n}_\rho$ and $\hat{n}_z$ are shown in Fig. 9, Appendix E.

Expanding the expressions in Eq (58) produces an integral-differential equation which has twenty-eight terms (see Appendix E). These terms, except for the source terms, can be easily separated into a product of z, ρ, μ and χ integrals. This is an integral separation of variables which is a direct result of Eq. (53); where, it is assumed that the solution can be expressed in a form where the dependent variables are separable. This separation property simplifies the individual integrals which have to be evaluated. It allows for the evaluation of only single integrals and not the more complicated double, triple or quadruple integrals. By this separation of variables it may be possible to integrate most of these single integrals analytically and thus avoid a numerical integration process.

The Spherical Harmonic Integrals. The use of a spherical harmonic angular trial function expansion was motivated by six basic considerations:

1. Because of the global nature of these functions the computational effort will be substantially reduced.

2. Spherical harmonics are well-known functions with orthonormal and symmetric (odd, even) properties.

3. The scattering cross sections are usually expanded in spherical harmonics (see Appendix A).

4. Spherical harmomics will produce a system of equations which are elliptic and invariant under continuous coordinate rotations (Ref 1:362).

5. An analytic or closed form evaluation of the angular integrals might be possible.

6. The even parity angular fluence, Eq (53), can be easily integrated to give the total particle fluence. This integration is carried out in Appendix I.

The term-by-term expansion of Eq (58) has been partly carried out in Appendix E. The resulting angle integrals are only dependent on the degree of the spherical harmonic trial function expansion which is used. They are not dependent on the problem parameters and therefore they can be independently evaluated. They can be evaluated once, and thereafter, used as a part of the problem input data.

Three approaches were pursued in an attempt to evaluate the angle integrals which are produced by this expansion. The first approach was to use the orthogonal properties of the associated Legendre functions and the well-known properties of sines and cosines to analytically evaluate these integrals. However, because of their complicated nature (see Appendix F) a closed form analytic integration was not easily obtained for most of them.

The second approach was to use a computer routine that can evaluate these integrals in a symbolic or algebraic sense. Such a routine will transform the integrals into algebraic expressions. The program Macysma which was written by the Massachusetts Institute of Technology Math Group was used in this attempt. However,

because of the time constraint on this research project and the need to learn a new programming language this approach was abandoned.

Finally, it was decided to evaluate these integrals by a numerical integration technique. Because it is possible to separate the integration variables, the computational effort can be substantially reduced by using a single (one variable) integration routine. So as to further reduce the computational effort, Eq (58) was completely expanded and twenty distinct angle integrals were identified. These integrals can be found in Appendix F. A ten point Newton-Cotes single integration routine was used to evaluate them. They were evaluated for each combination of the m, ℓ, k and n trial and weight function subscripts.

<u>Bicubic Polynomial Splines</u>. The spatial dependence of the particle fluence in the air-over-ground problem is approximated by a product of cubic splines. The use of cubic polynomial splines in the trial function expansion of Eq (53) requires the formation of a tensor product space. This space is made up of bicubic polynomial splines which are products of ρ and z-splines on a rectangular grid (Ref 15:131). The exact shape of these bicubic splines are obtained from a variational principle or the equivalent method of weighted residuals (<u>i.e.</u>, a solution of Eq (58)).

Bicubic polynomial splines are being used for the following reasons:

1. They are piecewise continuous and form a [illegible] such that the integral [illegible].

This reduces the number of integrals which must be evaluated and also produces a sparse and banded coefficient matrix.

2. A separation of the ρ and z integration variables is possible.

3. Third degree polynomials such as cubic splines have a faster rate of convergence than those of lower degree. Cubic splines are also twice continuously differentiable and thus they are very smooth functions. For a given problem mesh size splines will produce a coefficient (stiffness) matrix that is smaller but less sparse than hermites or lagrange polynomials.

The expansion of Eq (58) with a trial function of bicubic splines and spherical harmonics is carried out in Appendix E. A further expansion of these equations and a separation of the variables of integration produced seventeen distinct ρ and z integrals. These integrals which include the space source integrals are listed in Appendix G. The source integrals are derived from an interpolation of the first scatter source over the entire spatial problem domain.

<u>The Source Terms</u>. A numerical solution to the air-over-ground problem and the second order Boltzmann equation requires that the source terms (right hand side of Eq (58)) must be evaluated. These terms form the individual elements of the problem source vector in Eq (59). The even and odd parity sources S^g and S^u will be defined as the first scatter or collision even and odd parity sources. The first scatter source $S(\hat{r},\hat{\Omega})$ is the number density of particles which leave the burst point and undergo <u>only one</u> collision before being scattered into direction $\hat{\Omega}$ at position $\hat{r}$. Streaming neutrons which leave the burst point and do not collide before reaching position $(\hat{r},\hat{\Omega})$ are not included in the collision source.

The use of a first scatter source makes the air-over-ground problem more isotropic. It removes the strongly anisotropic streaming particles from being a part of the problem source. Therefore, the solution fluence of Eq (58) will be the scattered even parity fluence $\Psi_s(\hat{r},\hat{\Omega})$ and not the total even parity fluence $\Psi_t(\hat{r},\hat{\Omega})$. The total even parity fluence can be defined as

$$\Psi_t(\hat{r},\hat{\Omega}) = \Psi_s(\hat{r},\hat{\Omega}) + \Psi_d(\hat{r},\hat{\Omega}) \tag{63}$$

where

$\Psi_d(\hat{r},\hat{\Omega})$ = streaming uncollided particles at position $(\hat{r},\hat{\Omega})$.

A precise mathematical definition of the S^g and S^u sources will now be developed. Also a source interpolation procedure will be outlined. This source interpolation is used in order to simplify the source integrals of Appendix E (E-40 to E-46).

<u>The First Scatter Sour</u>. The even and odd parity sources have been defined as

$$S^u(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\{S(\hat{r},\hat{\Omega}) - S(\hat{r},-\hat{\Omega})\} \tag{10}$$

$$S^g(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\{S(\hat{r},\hat{\Omega}) + S(\hat{r},-\hat{\Omega})\} \tag{9}$$

If S^u and S^g are first scatter source densities then $S(\hat{r},\hat{\Omega})$ and $S(\hat{r},-\hat{\Omega})$ must also be defined as first scatter source particles/unit volume. If a position (ρ,z) in the problem domain is chosen then a unit vector from the burst point (0,zb) can be defined as

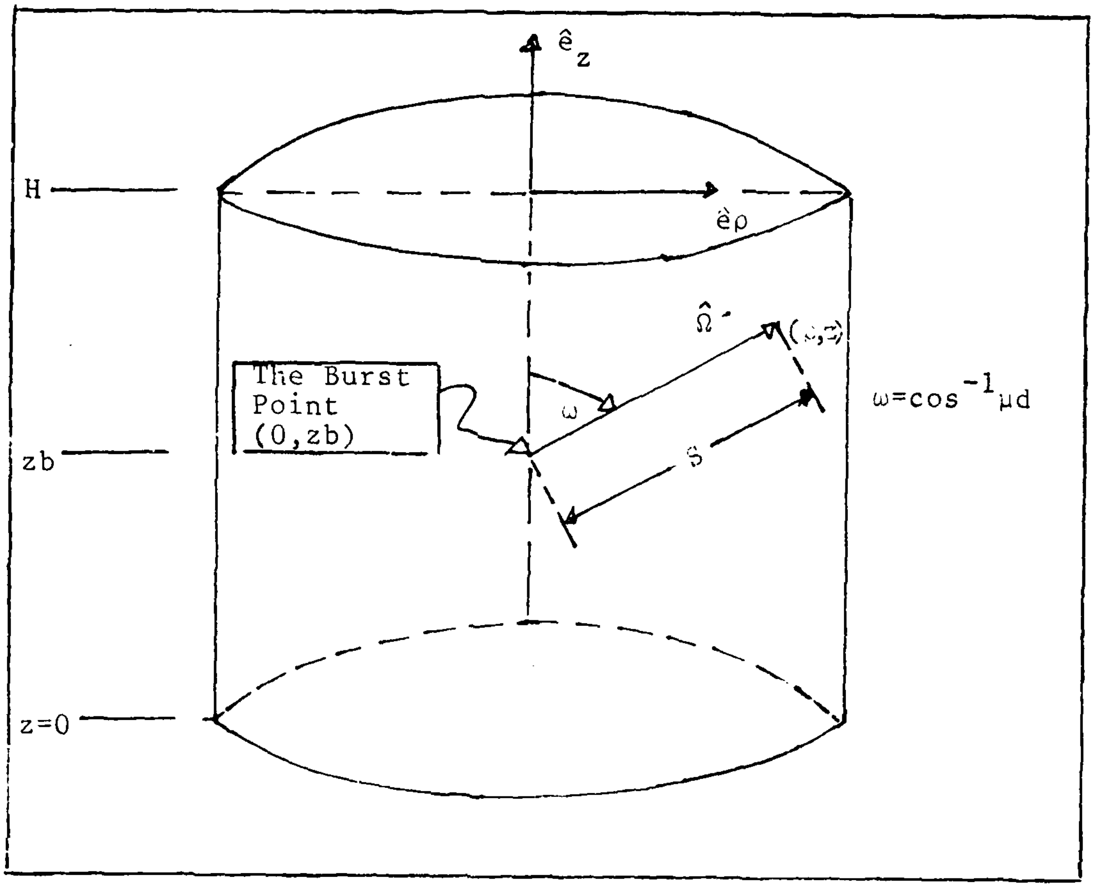

Figure 5. First Scatter (Collision) Source Direction Vectors

$$\hat{\Omega}'(\rho,z) = \frac{\rho\hat{e}_\rho + (z-zb)\hat{e}_z}{\{\rho^2 + (z-zb)^2\}^{\frac{1}{2}}} \tag{64}$$

Fig. 5 shows the direction vectors of this first scatter (collision) source. $\hat{\Omega}'$ is the direction that all streaming (uncollided) particles have at point (ρ,z).

By definition only particles which are streaming radially outward from the burst point can be included in the direct fluence. Therefore the direct fluence at point (ρ,z) is in the $\hat{\Omega}'$ direction and can be written as

$$\phi_d(\rho, z, \hat{\Omega}') = \frac{Y}{4\pi S^2} \exp\{-\int_0^s \sigma_t(z)ds\} \quad , \tag{65}$$

where

$$s = \{\rho^2 + (z-zb)^2\}^{\frac{1}{2}} \tag{66}$$

and $\int ds$ means that the integration is carried out along the path s (see Fig. 5). Also

Y = Total particle yield of the nuclear explosion at the burst point.

$$\sigma_t(z) = \begin{cases} \sigma_t(0)e^{-z/sh} & \text{for } z > 0 \\ \sigma_t \text{ (ground)} & \text{for } z < 0 \end{cases} \tag{67}$$

sh = atmospheric scale height

The term $\int_0^s \sigma_t(z)ds$ is the average number of collisions which a particle undergoes in traveling from the burst point (o, zb) to point (ρ, z). From Fig. 5 the distance s can also be written as

$$s = (z-zb)/\mu d \tag{68}$$

and therefore by changing variables

$$ds = dz/\mu d \tag{69}$$

where μd is a function of ρ and z (but constant along a path length S)

$$\mu d(\rho, z) = \cos \omega = (z-zb)/s = (z-zb)/\{\rho^2 + (z-zb)^2\}^{\frac{1}{2}} \tag{70}$$

The integral term of Eq (65) can now be written for $z > 0$ as

$$\tau(\rho, z) = \int_0^s \sigma_t(z)ds = \frac{\sigma_t(o)}{\mu d}\int_{zb}^{z} e^{-z/sh}dz \tag{71}$$

and finally as

$$\tau(\rho,z) = \frac{\sigma_t(o)}{\mu d}\{e^{-zb/sh} - e^{-z/sh}\}\cdot sh$$

$$= \{\sigma_t(zb) - \sigma_t(z)\}\cdot\frac{sh}{\mu d} \tag{72}$$

From the above derivation it follows that

$$\tau(\rho,z) = \begin{cases} \{\sigma_t(zb) - \sigma_t(z)\}\cdot sh/\mu d \text{ for } z > 0 \\ \{\sigma_t(zb) - \sigma_t(0)\}\cdot sh/\mu d - \sigma_t z/\mu d \text{ for } z < 0 \end{cases} \tag{73}$$

also

$$\phi_d(\rho,z,\hat{\Omega}') = \frac{Y}{4\pi S^2}\exp(-\tau(\rho,z)) \tag{74}$$

Note that $\phi_d(\rho,z,\hat{\Omega}')$ is only a function of ρ and z.

The first scatter source at (ρ,z) and with direction $\hat{\Omega}$ are those particles which undergo their first collision at (ρ,z) and are scattered from direction $\hat{\Omega}'$ to $\hat{\Omega}$. Therefore the first scatter source can now be defined as

$$S(\rho,z,\hat{\Omega}) = \sigma^s(z,\hat{\Omega}\cdot\hat{\Omega}')\phi_d(\rho,z,\hat{\Omega}') \tag{75}$$

where σ^s is not a function of $\hat{\Omega}'$ but of the scattering angle $\hat{\Omega}\cdot\hat{\Omega}'$ (μ_o) and z. From Fig. 5 and Fig. 2 $\hat{\Omega}'$ is defined by μd and $\chi = 0$ i.e. $\hat{\Omega}' = (\mu',\chi')$ where $\mu' = \mu d$ and $\chi' = 0$.

By use of the addition theorem it is shown in Appendix H that Eq (75) can be written as

$$S(\rho,z,\hat{\Omega}) = 2\phi_d(r,z,\hat{\Omega}')e^{-z/sh}\sum_{\ell=0}^{L}\sum_{m=0}^{\ell}\sigma_\ell^s(0)C_{\ell m}^2 P_{\ell m}(\mu)P_{\ell m}(\mu d)\cos m\chi \tag{76}$$

and that the even and odd parity first scatter sources are

$$S^g(\rho,z,\hat{\Omega}) = \phi_d(\rho,z,\hat{\Omega}')e^{-z/sh}\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma_\ell^s(0)C_{\ell m}^2\{1+(-1)^{\ell-m}\}P_{\ell m}(\mu d)P_{\ell m}(\mu)\cos m\chi \tag{77}$$

and

$$S^u(\rho,z,\hat{\Omega}) = \phi_d(\rho,z,\hat{\Omega}')e^{-z/sh}\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma_\ell^s(0)C_{\ell m}^2\{1-(-1)^{\ell-m}\}P_{\ell m}(\mu d)P_{\ell m}(\mu)\cos m\chi \tag{78}$$

where m^* means that all terms with a m = 0 subscript must be divided by two, and $\cos m\chi$ should be interpreted as cosine $(m\chi)$

<u>Source Interpolation</u>. Because of the complicated nature of the source expressions, Eqs (77) and (78), and the need to integrate the source terms of Appendix E, a spatial source interpolation will be used. This interpolation which simplifies the source integrals is necessary if a very tedious (double or quadruple) integration is to be avoided. By this interpolation process the source terms of Appendix E can all be separated into a product of single integrals.

It is important to note that μd which is given by Eq (70) is a function of ρ and z and therefore $P_{\ell m}(\mu d)$ is also a function of ρ and z. Furthermore $\phi_d(\rho,z,\hat{\Omega}')$ of Eq (74) is a function of ρ and z. Beginning with Eqs (77) and (78) they can be rewritten as

$$S^g(\rho,z,\hat{\Omega}) = \sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma_\ell^s(0)C_{\ell m}^2\{1+(-1)^{\ell-m}\}A_{\ell m}(\rho,z)P_{\ell m}(\mu)\cos m\chi \tag{79}$$

and

$$S^u(\rho,z,\hat{\Omega}) = \sum_{\ell=0}^{L}\sum_{m=0}^{\ell} \sigma_\ell^s(0) C_{\ell m}^2 \{1-(-1)^{\ell-m}\} A_{\ell m}(\rho,z) P_{\ell m}(\mu)\cos m\chi \tag{80}$$

where

$$A_{\ell m}(\rho,z) = \phi_d(\rho,z,\hat{\Omega}')P_{\ell m}(\mu d)e^{-z/sh} \tag{81}$$

A spatial (ρ,z) interpolation of the even and odd parity sources, Eqs (79) and (80), is therefore an interpolation of $A_{\ell m}(\rho,z)$. In this project these first scatter second order sources were interpolated by a combination of piecewise bi-linear Lagrange polynomial functions. Specifically, S^g was approximated by a tensor product of linear Lagrange polynomials as follows

$$S^g(\rho,z,\hat{\Omega}) = \sum_{i=1}^{NZ}\sum_{j=1}^{NR} S^g(\rho_j,z_i,\hat{\Omega})H_j(\rho)H_i(z) \tag{82}$$

where

$S^g(\rho_j,z_i,\hat{\Omega})$ = the even parity source, Eq (79) evaluated at the spacial nodes (ρ_j,z_i)

NZ = total number of z-nodes

NR = total number of R-nodes

$H(\rho)$ = ρ-linear Lagrange polynomial

$H(z)$ = z-linear Lagrange polynomial

These linear polynomials are defined as

$$H_i(x) = \begin{cases} \dfrac{x_{i-1}-x}{x_{i-1}-x_i}, & x_{i-1}\le x\le x_i \end{cases} \quad \text{and} \quad H_i(x) = \begin{cases} \dfrac{x_{i+1}-x}{x_{i+1}-x_i}, & x_i\le x\le x_{i+1} \end{cases} \tag{83}$$

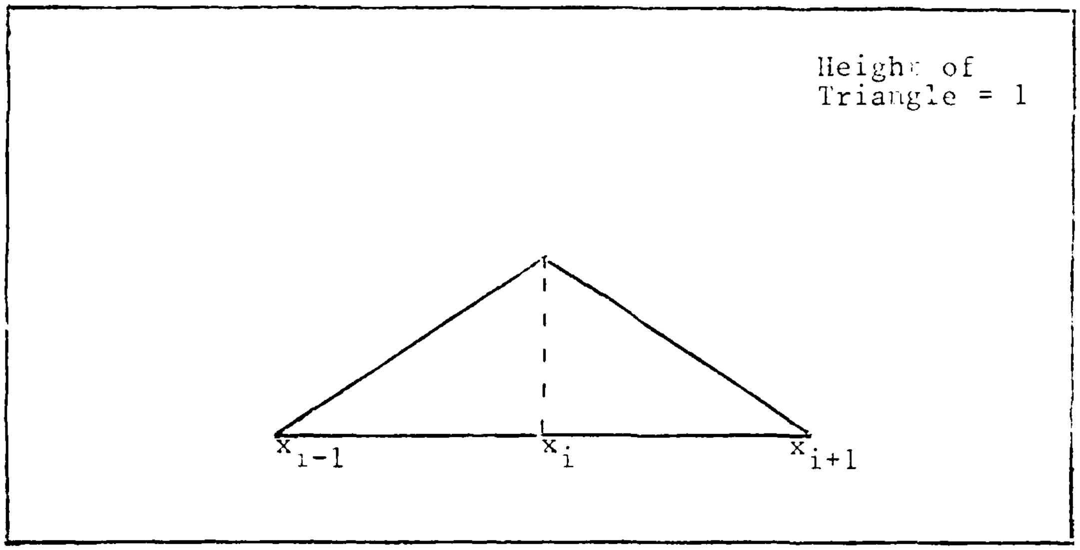

Figure 6. A Linear Lagrange Polynomial Function.

The product $H_j(\rho)\cdot H_i(z)$ of Eq (82) forms a tensor product space on a rectangular grid, in the ρ, z plane (Ref 15:129)

Substituting Eq (82) for $S^g(\rho_j, z_i, \hat{\Omega})$ in Eq (77) gives

$$S^g(\rho,z,\hat{\Omega}) = \sum_{\ell=0}^{L} \sum_{m=0}^{\ell} \Big[P_\ell^m(0) C^2_{\ell m} \{1 + (-1)^{\ell-m}\} P_{\ell m}(\mu) \cos m\chi \sum_{i=1}^{NZ} \sum_{j=1}^{NR} A_{\ell m}(\rho_j, z_i) H_j(\rho) H_i(z) \Big] \tag{84}$$

Similarly the odd parity source can also be expressed as

$$S^u(\rho,z,\hat{\Omega}) = \sum_{\ell=0}^{L} \sum_{m=0}^{\ell} \Big[P_\ell^m(0) C^2_{\ell m} \{1 - (-1)^{\ell-m}\} P_{\ell m}(\mu) \cos m\chi \sum_{i=1}^{NZ} \sum_{j=1}^{NR} A_{\ell m}(\rho_j, z_i) H_j(\rho) H_i(z) \Big] \tag{85}$$

Eqs (84) and (85) can now be substituted into the source terms of Appendix E (E-40 to E-46). This substitution and a separation of the integration variables produced six distinct space integrals. These space integrals are listed in Appendix

G. The source angle integrals have been included in those integrals which are presented in Appendix F.

V Computer Implementation and Results

A numerical solution of the air-over-ground problem can be obtained from a computer solution of the system of coupled algebraic equations which are represented by Eq (58). These equations can be written in the matrix form of Eq (59) and through a direct inversion or some other matrix solution process the $A_{i,j,\ell,m}$ mixing coefficients can be found.

The computer solution to this problem was accomplished by a two step process. Each element of the stiffness matrix and source vector was computed and assembled in the matrix form of Eq (59). Then the mixing coefficients were computed by the iterative matrix solution method of successive over-relaxation. An indirect iterative matrix solution method is possible because Eq (58) and the stiffness matrix of Eq (59) is symmetric positive definite. A computer program which assembles the problem matrices and computes the mixing coefficients and particle fluences was written. This program which is written in FORTRAN V is listed in Appendix J.

Using a ten point Newton-Cotes numerical integration routine, each of the thirty-seven integrals in Appendix F and G were evaluated. The angular integrals were evaluated for each ℓm, kn combination of the trial and weight function subscripts. Selected products of these integrals were then used to generate each of the twenty-eight terms (E-19 to E-46) of Appendix E. Following the prescription of Appendix

E the first twenty-one terms were then added (or subtracted) to produce the elements of the *stiffness matrix*. The next seven terms gave the elements of the source vector.

Writing the synthesized Boltzmann equation, Eq (58), in operator notation as

$$L(\Psi_{\substack{iz,ir\\ \ell,m}})\eta_{\substack{jz,jr\\ k,n}} = S\eta_{\substack{jz,jr\\ k,n}} \tag{86}$$

where Ψ and η are defined by Eqs (53) and (55) and

$$L(\Psi_{\substack{iz,ir\\ \ell,m}})\eta_{\substack{jz,jr,\\ k,n}} = \text{Left hand side of Eq (58)}$$

$$S\eta_{\substack{jz,jr\\ k,n}} = \text{Right hand side of Eq (58)}$$

the $K_{p,q}$ element of the stiffness matrix is

$$K_{p,q} = L\{B_{iz}(z)B_{ir}(\rho)Q_{\ell m}\}\cdot B_{jz}(z)B_{jr}(\rho)Q_{kn} \tag{87}$$

where

$$q = (m+1) + \frac{\ell(\ell+1)}{2} + \frac{(Lmax + 1)(Lmax + 2)}{2}\cdot\{(ir-1) + IR(iz-1)\} \tag{88}$$

and

$$p = (n+1) + \frac{k(k+1)}{2} + \frac{(Lmax + 1)(Lmax + 2)}{2}\cdot\{(jr-1) + JR(jz-1)\} \tag{89}$$

The corresponding source vector element S_p is given by

$$S_p = S\cdot B_{jz}(z)B_{jr}(\rho)Q_{kn} \tag{90}$$

where p is given by Eq (89) and

Lmax = degree of the spherical harmonic expansion

JR=IR = total number of ρ-splines

p = the row index of the problem (K) matrix

q = column index of matrix K

$B(z)$, $B(\rho)$ and $Q_{\ell m}$ are defined in Chapter IV (Eqs (50) and (54)). iz, ir, jr, jz, ℓ, m, k, and n are the trial and weight function expansion subscripts where

ℓ,k = 0 to Lmax

m = 0 to ℓ,

n = 0 to k

iz,jz = 1 to IZ

ir,jr = 1 to IR

and

IZ = total number of z-splines

IR = total number of ρ-splines

Using the notation of Eqs (87), (88) and (89) the K-problem matrix and S-source vector can be easily assembled in the following do loop.

```
DO 10 jz = 1, IZ
DO 10 jr = 1, IR
DO 10  k = 0, Lmax
DO 10  n = 0, k
       S_p = S*n_iz,jr,k,n
DO 10 iz = 1, IZ
DO 10 ir = 1, IR
DO 10  ℓ = 0, Lmax
DO 10  m = 0,ℓ
```

$$K_{p,q} = L(\Psi_{\substack{iz,ir \\ \ell,m}}) \, \eta_{\substack{jz,jr \\ k,n}}$$

10 continue

The assembled coefficient (K) matrix which results from Eq (58) and a bicubic spline spherical harmonic trial function expansion is sparse and symmetric. Because of this symmetry and sparseness the coefficient matrix can be stored within the computer by special storage schemes (Ref 14:70). These sparse and symmetric schemes will greatly reduce the computer storage requirements. As an example, in a trial function expansion where JR = IR = 8 and Lmax = 2 the problem coefficient matrix is a 384 x 384 square symmetric matrix with many elements which are zero. Therefore if this entire matrix is stored within the computer it will req. e 147456 separate storage locations. This much core storage is already beyond the capacity of most computers. However, by using a sparse and symmetric storage scheme this matrix can be reduced to one with less than 73728 elements. For large trial function expansions (JR = IR = 50, Lmax = 3), special auxiliary storage and solution techniques will be necessary.

This entire problem (coefficient and source matrices) was assembled on a CDC 6600 computer at the Air Force Institute of Technology. The 384 x 384 problem matrix is too large to be stored in core memory unless a sparse symmetric storage mode is used. Because some of the (ρ) integrals in Appendix G are discontinuous (infinite) at

$\rho = 0$ it was necessary to use a lower ρ-integration limit of 1.0 E-8. Also, since the first scatter sources of Eqs (77) and (78) are undefined at the burst point none of the problem nodes can be located there (see Fig. 5).

Results

The computer routines which are listed in Appendix J were used to produce a numerical solution to the air-over-ground problem. These routines demonstrate the feasibility of using FESAS to produce a computer solution to the two-dimensional steady state anisotropic Boltzmann equation. This computer program has not been fully developed, refined or debugged and therefore the accuracy of the results has not been evaluated. These results are presented in an attempt to further show that FESAS is a viable numerical solution technique.

The problem domain is a cylinder which sits on the surface of the earth (see Fig. 5). However, the air-ground interface is not included in the problem domain and therefore all ground effects are ignored. The following problem parameters were used

Weapon yield = 1.0E+23 neutrons

Cylinder height = .4km

Cylinder radius = .4km

Burst height = .12 km

Total cross section ($\sigma_t(0)$) = 15.0 km^{-1}

Table I

Legendre Expansion Coefficients which were used in a Numerical Solution of the Air-Over-Ground Problem

Expansion subscript ℓ	Legendre expansion coefficients	
	σ_ℓ^g	σ_ℓ^u
0	10.0	.0
1	0.0	2.5

The cross-sections in Table I were arbitrarily chosen and they do not represent the actual values for air at sea level. A relative convergence criteria (.001) which is accurate to three significant figures was used.

The program execution times varied with the degree of the spherical harmonic trial function expansion and the problem mesh (grid) size. The entire problem matrices were stored within core memory and by trial and error it was determined that a relaxation parameter of 1.7 gave the fastest convergence rate. However, as more trial functions were used and the system of equations and matrices grew larger the rate of convergence decreased. In Table II the program execution times and the number of iterations to convergence are listed for various problem mesh sizes. These execution times and convergence rates can be substantially reduced by rewriting or modifying the program routines of Appendix J.

Table II

Execution Times and Convergence Rates for the FESAS Computer Code

Spatial Grid	Degree (Lmax) of the Spherical Harmonic Trial Function Expansion	Execution Times (secs)	Number of Iterations to Convergence
1x1	0	47.8	1395
1x1	1	351.754	2001
2x2	0	60.315	785
2x2	1	361.3	801
4x4	0	79.62	265
4x4	1	816.7	492
8x8	0	236.83	168

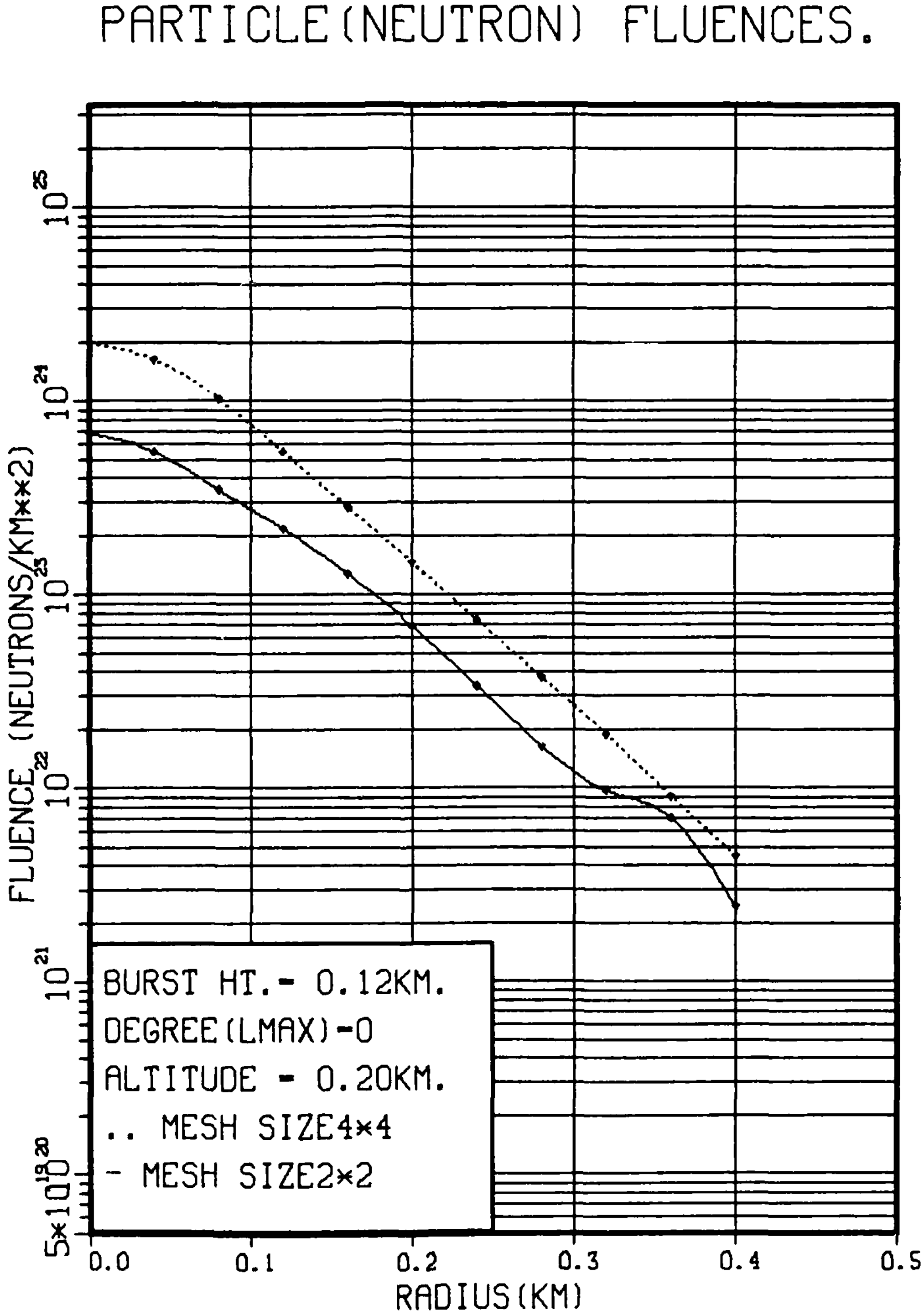

Figure 7. Computed Fluences as a Function of Radius and showing a variation with the Problem Spatial Mesh Size.

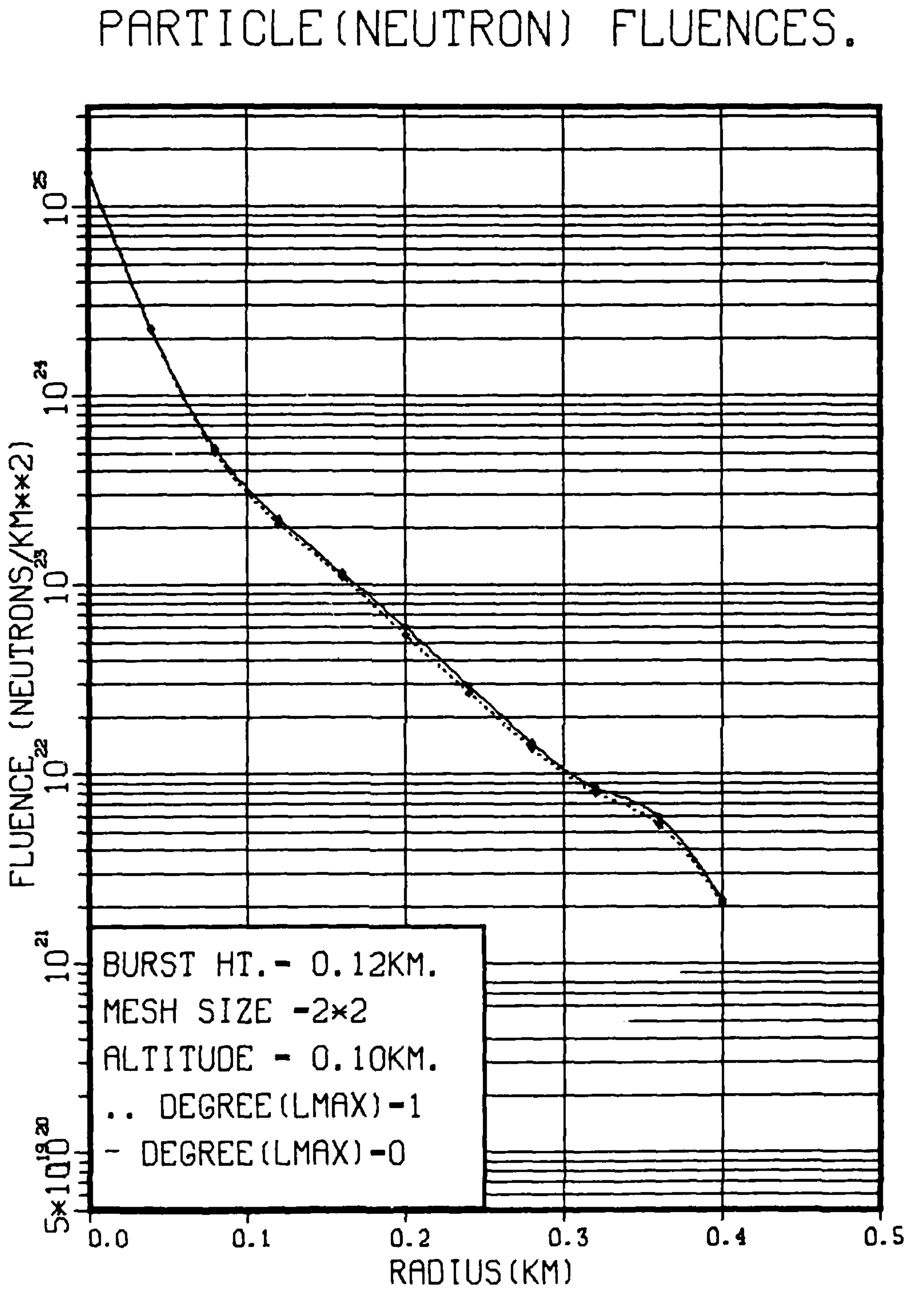

Figure 8. Computed Fluences as a Function of Radius and showing a variation with the Degree of the Angular Spherical Harmonic Trial Function Expansion.

In Figures 7 and 8 fluence values as a function of radius are presented. These values are representative of an altitude of 200 metres and the aforementioned problem parameters. Figure 7 shows a variation of the solution with spatial grid (mesh) sizes whereas Figure 8 shows a variation with the degree of the spherical harmonic trial function expansion. More detailed numerical results can be found in Appendix K.

VI Conclusions and Recommendations

Conclusions

A finite element space-angle synthesis (FESAS) solution of the steady state anisotropic Boltzmann equation in two-dimensional cylindrical geometry has been presented. In this presentation a weak form of the even parity steady state Boltzmann equation was developed. It was shown that because the problem equations were positive definite and self-adjoint the Rayleigh-Ritz variational principle and the Bubnov-Galerkin method of weighted residuals are equivalent. The problem solution was formulated by using a trial function expansion in bicubic polynomial splines and spherical harmonics. This trial function expansion has a dual basis -- a local basis in space and a global basis in angle.

This development was specialized to the air-over-ground neutral particle transport problem. It was shown that a finite element space-angle synthesis solution is possible and that a first scatter interpolation source can be used. It was also shown that a numerical solution can be achieved and that this solution technique may eliminate ray effects and reduce computational costs.

Recommendations

The preliminary results of this study have shown that the FESAS method can produce a numerical solution to the steady state Boltzmann equation and the air-over-ground problem. However, because of the time constraints on this

research project a complete development and evaluation of the FESAS method was not accomplished. Therefore, there are a number of recommendations for the further analysis and evaluation of the FESAS method, which must be made. Some of these recommendations are:

1. To enforce the boundary conditions at the air-over-ground interface. This can be accomplished by a coalescing or stacking of the nodes (knots) of the bicubic splines and by using a Double-P_N approximation at this interface.

2. Develop or refine the computer algorithm so that a comparative study can be made. This study should include a comparison of the computational costs and accuracy of FESAS to those of Monte Carlo and discrete ordinates. Also, a determination should be made as to whether ray effects have been eliminated.

3. Obtain, if possible, a closed form solution to the angle integrals in Appendix F.

4. Explore other ways of handling the discontinuity (at $\rho = 0$) of the space integrals.

5. Use other spatial trial functions. Lower degree bi-quadratic splines, hermites and Lagrange polynomials are possible candidates. A comparison of the results which are obtained from the use of various trial functions can then be made.

6. Examine the effects of an improved source interpolation on the solution accuracy and rate of convergence. An improved source interpolation can be achieved by the use of a smaller source (space) grid or a higher degree Lagrange or Hermite polynomial interpolation function

7. Extend the use of finite element space-angle synthesis to the solution of energy dependent multi-group problems.

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Appendix A

Derivation of the Scattering Kernel, Inverse Collision Operators and the Even and Odd Parity Collision Cross Sections

Collision Cross-Sections

The even and odd parity legendre expansion scattering cross-sections σ_ℓ^g and σ_ℓ^u originate in the derivation of the second order forms of the Boltzman equation (Chapter III). A definition of these quantities has been given elsewhere (Ref 5:29). This definition is repeated below.

Beginning with the even and odd parity scattering cross sections

$$\sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') = \frac{1}{2}\left\{\sigma^s(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') + \sigma^s(\hat{r},-\hat{\Omega}\cdot\hat{\Omega}')\right\} \quad \text{(A-1)}$$

$$\sigma_s^u(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') = \frac{1}{2}\left\{\sigma^s(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') - \sigma^s(\hat{r},-\hat{\Omega}\cdot\hat{\Omega}')\right\} \quad \text{(A-2)}$$

the usual computational practice (Ref 6:131) is to expand these scattering cross sections in Legendre polynomials as

$$\sigma^s(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') = \sum_{\ell=0}^{L} \sigma_\ell^s(\hat{r}) \cdot \frac{2\ell+1}{4\pi} \cdot P_\ell(\hat{\Omega}\cdot\hat{\Omega}') \quad \text{(A-3)}$$

or

$$\sigma^s(\hat{r},-\hat{\Omega}\cdot\hat{\Omega}') = \sum_{\ell=0}^{L} \sigma_\ell^s(\hat{r}) \cdot \frac{2\ell+1}{4\pi} \cdot P_\ell(-\hat{\Omega}\cdot\hat{\Omega}') \quad \text{(A-4)}$$

where

$\sigma^s(r,\hat{\Omega}\cdot\hat{\Omega}')$ = macroscopic scattering cross section

$\sigma_\ell^s(r)$ = Legendre macroscopic cross-section expansion coefficient which is a function of position (material)

L = the degree Legendre polynomial expansion which is used

$P_\ell(\Omega\cdot\Omega')$ = Legendre polynomial of degree ℓ.

$\hat{\Omega}\cdot\hat{\Omega}'$ = scattering angle (μ_o = Cosθ)

Inserting Eqs (A-3) and (A-4) into (A-1) and (A-2) gives

$$\sigma_s^g(\bar{r},\hat{\Omega}.\hat{\Omega}') = \frac{1}{2}\sum_{\ell=0}^{L}\sigma_\ell^s(r)\,\frac{2\ell+1}{4\pi}\left\{P_\ell(\hat{\Omega}.\hat{\Omega}') + P_\ell(-\hat{\Omega}.\hat{\Omega}')\right\} \tag{A-5}$$

$$\sigma_s^u(\bar{r},\hat{\Omega}.\hat{\Omega}') = \frac{1}{2}\sum_{\ell=0}^{L}\sigma_\ell^s(r)\,\frac{2\ell+1}{4\pi}\left\{P_\ell(\hat{\Omega}.\hat{\Omega}') - P_\ell(-\hat{\Omega}.\hat{\Omega}')\right\} \tag{A-6}$$

From the even and odd properties of Legendre polynomials (Ref 17:223)

$$P_\ell(\hat{\Omega}.\hat{\Omega}') = \begin{cases} \text{even function if } \ell \text{ is even} \\ \text{odd function if } \ell \text{ is odd} \end{cases} \tag{A-7}$$

therefore

$$\sum_{\ell=0}^{L}\left\{P_\ell(\hat{\Omega}.\hat{\Omega}') + P_\ell(-\hat{\Omega}.\hat{\Omega}')\right\} = \begin{cases} 0 & \text{if } \ell \text{ is odd} \\ 2P_\ell(\hat{\Omega}.\hat{\Omega}') & \text{if } \ell \text{ is even} \end{cases} \tag{A-8}$$

and

$$\sum_{\ell=0}^{L}\left\{P_\ell(\hat{\Omega}.\hat{\Omega}') - P_\ell(-\hat{\Omega}.\hat{\Omega}')\right\} = \begin{cases} 2P_\ell(\hat{\Omega}.\hat{\Omega}') & \text{if } \ell \text{ is odd} \\ 0 & \text{if } \ell \text{ is even} \end{cases} \tag{A-9}$$

Eqs (A-5) and (A-6) can now be rewritten as

$$\sigma_s^g(\bar{r},\hat{\Omega}.\hat{\Omega}') = \sum_{\substack{\ell=0 \\ \ell \text{ even}}}^{L}\sigma_\ell^s(r)\,\frac{2\ell+1}{4\pi}\,.\,P_\ell(\hat{\Omega}.\hat{\Omega}') \tag{A-10}$$

and

$$\sigma_s^u(\bar{r},\hat{\Omega}.\hat{\Omega}') = \sum_{\substack{\ell=1 \\ \ell \text{ odd}}}^{L}\sigma_\ell^s(r)\,\frac{2\ell+1}{4\pi}\,.\,P_\ell(\hat{\Omega}.\hat{\Omega}') \tag{A-11}$$

The even and odd parity cross-sections can also be expanded in Legendre polynomials as

$$\sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') = \sum_{\ell=0}^{L} \sigma_\ell^g(\hat{r})\cdot\frac{2\ell+1}{4\pi}\cdot P_\ell(\hat{\Omega}\cdot\hat{\Omega}') \tag{A-12}$$

and

$$\sigma_s^u(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') = \sum_{\ell=0}^{L} \sigma_\ell^u(\hat{r})\cdot\frac{2\ell+1}{4\pi}\cdot P_\ell(\hat{\Omega}\cdot\hat{\Omega}') \tag{A-13}$$

Comparing Eqs (A-13), (A-12), (A-11) and (A-10) it is apparent that

$$\sigma_\ell^g(\hat{r}) = \begin{cases} \sigma_\ell^s(\hat{r}) & \text{for } \ell \text{ even} \\ 0 & \text{for } \ell \text{ odd} \end{cases} \tag{A-14}$$

and

$$\sigma_\ell^u(\hat{r}) = \begin{cases} 0 & \text{for } \ell \text{ even} \\ \sigma_\ell^s(\hat{r}) & \text{for } \ell \text{ odd} \end{cases} \tag{A-15}$$

Therefore $\sigma_\ell^g(\hat{r})$ and $\sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')$ are even functions. Also $\sigma_\ell^u(\hat{r})$ and $\sigma_s^u(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')$ are odd functions.

Scattering Kernel

In the development of the even and odd parity forms of the anisotropic steady state Boltzmann equation (Chapter III), it was necessary to express the scattering kernels in terms of the even and odd parity flux (fluence) components. Following the derivation of Wheaton (Ref 5:11) the scattering terms can be written as

$$\int_{4\pi} \sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\,\phi(\hat{r},\hat{\Omega}')\,d\hat{\Omega}' = \frac{1}{2}\int_{4\pi} \sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\,\phi(\hat{r},\hat{\Omega}')\,d\hat{\Omega}' + \frac{1}{2}\int_{4\pi} \sigma_s^g(\hat{r},\hat{\Omega}\cdot-\hat{\Omega}')\,\phi(\hat{r},-\hat{\Omega}')\,d\hat{\Omega}' \tag{A-16}$$

where the integrations are carried out over all directions.

Because σ_s^g is an even function, meaning f(x) = f(-x), it follows that

$$\sigma_s^g(\hat{r},\hat{\Omega}\cdot-\hat{\Omega}') = \sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') \tag{A-17}$$

and therefore

$$\int_{4\pi}\sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\phi(\hat{r},\hat{\Omega}')d\hat{\Omega}' = \frac{1}{2}\int_{4\pi}\sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\{\phi(\hat{r},\hat{\Omega}') + \phi(\hat{r},-\hat{\Omega}')\}d\hat{\Omega}' \tag{A-18}$$

With the even parity flux defined as

$$\psi(\hat{r},\hat{\Omega}') = \frac{1}{2}\{\phi(\hat{r},\hat{\Omega}') + \phi(\hat{r},-\hat{\Omega}')\} \tag{A-19}$$

Eq (A-18) becomes

$$\int_{4\pi}\sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\phi(\hat{r},\hat{\Omega}')d\hat{\Omega}' = \int_{4\pi}\sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\psi(\hat{r},\hat{\Omega}')d\hat{\Omega}' \tag{A-20}$$

and by a similar derivation

$$\int_{4\pi}\sigma_s^u(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\phi(\hat{r},\hat{\Omega}')d\hat{\Omega}' = \int_{4\pi}\sigma_s^u(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')\chi(\hat{r},\hat{\Omega}')d\hat{\Omega}' \tag{A-21}$$

<u>Inverse Collision Operators</u>

In deriving the second order forms of the Boltzmann equation (Chapter III) the G^g and G^u operators were defined as

$$G^g f(\hat{\Omega}) = \sigma_t f(\hat{\Omega}) - \int_{4\pi}\sigma_s^g(\hat{\Omega}\cdot\hat{\Omega}')f(\hat{\Omega}')d\hat{\Omega}' \tag{A-22}$$

and

$$G^u f(\hat{\Omega}) = \sigma_t f(\hat{\Omega}) - \int_{4\pi}\sigma_s^u(\hat{\Omega}\cdot\hat{\Omega}')f(\hat{\Omega}')d\hat{\Omega}' \tag{A-23}$$

where the $\hat{r}$ dependence has been omitted in an attempt to simplify the notation.

Using the addition theorem (Ref 6:609)

$$P_\ell(\hat{r}\cdot\hat{r}') = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{+\ell} Y^*_{\ell m}(\hat{r}')\,Y_{\ell m}(\hat{r}) \tag{A-24}$$

in (A-12) and (A-13) gives

$$G_s^g(\hat{r}\cdot\hat{r}') = \sum_{\ell=0}^{L}\sum_{m=-\ell}^{+\ell} G_\ell^g\, Y^*_{\ell m}(\hat{r}')\,Y_{\ell m}(\hat{r}) \tag{A-25}$$

and

$$G_s^u(\hat{r}\cdot\hat{r}') = \sum_{\ell=0}^{L}\sum_{m=-\ell}^{+\ell} G_\ell^u\, Y^*_{\ell m}(\hat{r}')\,Y_{\ell m}(\hat{r}) \tag{A-26}$$

Eqs (A-22) and (A-23) can now be written as

$$G^g f(\hat{r}) = G_t f(\hat{r}) - \sum_{\ell=0}^{L}\sum_{m=-\ell}^{+\ell} G_\ell^g\, Y_{\ell m}(\hat{r}) \int_{4\pi} Y^*_{\ell m}(\hat{r}')\, f(\hat{r}')\, d\hat{r}' \tag{A-27}$$

and

$$G^u f(\hat{r}) = G_t f(\hat{r}) - \sum_{\ell=0}^{L}\sum_{m=-\ell}^{+\ell} G_\ell^u\, Y_{\ell m}(\hat{r}) \int_{4\pi} Y^*_{\ell m}(\hat{r}')\, f(\hat{r}')\, d\hat{r}' \tag{A-28}$$

The inverse operators are defined as

$$K^g = \left[G^g\right]^{-1} \quad \text{and} \quad K^u = \left[G^u\right]^{-1} \tag{A-29}$$

where it is meant that if

$$G^g f(\hat{r}) = R(\hat{r}) \tag{A-30}$$

then

$$K^g\left[G^g f(\hat{r})\right] = K^g R(\hat{r}) = f(\hat{r}) \tag{A-31}$$

multiplying Eq (A-30) by $\int_{4\pi} Y^*_{kn}(\hat{\Omega})d\hat{\Omega}$ and expanding the C^g operator gives

$$\sigma_t \int_{4\pi} f(\hat{\Omega}) Y^*_{kn}(\hat{\Omega}) d\hat{\Omega} - \sum_{\ell,m} \sigma^g_\ell \int_{4\pi} Y_{\ell m}(\hat{\Omega}) Y^*_{kn}(\hat{\Omega}) d\hat{\Omega} \int_{4\pi} Y^*_{\ell m}(\hat{\Omega}') f(\hat{\Omega}') d\hat{\Omega}'$$

$$= \int_{4\pi} R(\hat{\Omega}) Y^*_{kn}(\hat{\Omega}) d\hat{\Omega} \qquad \text{(A-32)}$$

using the orthonormal properties of spherical harmonics (Ref 6:609)

$$\int_{4\pi} Y_{\ell m}(\hat{\Omega}) Y^*_{kn}(\hat{\Omega}) d\hat{\Omega} = \delta_{\ell k}\delta_{mn} \qquad \text{(A-33)}$$

where $\delta_{\ell k}$ is the Kronecker delta which is defined by

$$\delta_{\ell k} = \begin{cases} 0 & \ell \neq k \\ 1 & \ell = k \end{cases} \qquad \text{(A-34)}$$

Therefore Eq (A-32) can now be written as

$$\sigma_t \int_{4\pi} f(\hat{\Omega}) Y^*_{kn}(\hat{\Omega}) d\hat{\Omega} - \sigma^g_\ell \int_{4\pi} Y^*_{kn}(\hat{\Omega}') f(\hat{\Omega}') d\hat{\Omega}'$$

$$= \int_{4\pi} R(\hat{\Omega}) Y^*_{kn}(\hat{\Omega}) d\hat{\Omega} \qquad \text{(A-35)}$$

and

$$\int_{4\pi} f(\hat{\Omega}) Y^*_{kn}(\hat{\Omega}) d\hat{\Omega} = \frac{1}{\sigma_t - \sigma^g_\ell} \int_{4\pi} R(\hat{\Omega}) Y^*_{kn}(\hat{\Omega}) d\hat{\Omega} \qquad \text{(A-36)}$$

Rewriting Eq (36) with a ℓm spherical harmonic subscript and substituting into the expanded form of Eq (A-30) gives

$$R(\hat{\Omega}) = \sigma_t f(\hat{\Omega}) - \sum_{\ell,m} \left\{ \frac{\sigma^g_\ell}{\sigma_t - \sigma^g_\ell} \right\} Y_{\ell m}(\hat{\Omega}) \int_{4\pi} R(\hat{\Omega}') Y^*_{\ell m}(\hat{\Omega}') d\hat{\Omega}' \qquad \text{(A-37)}$$

and by rearranging Eq (A-37)

$$f(\hat{r}) = \frac{1}{\sigma_t}\left[R(\hat{r}) + \sum_{\ell,m}\left\{\frac{\sigma_\ell^g}{\sigma_t - \sigma_\ell^g}\right\} Y_{\ell m}(\hat{r})\int_{4\pi} R(\hat{r}')Y_{\ell m}^*(\hat{r}')d\hat{r}'\right] \qquad \text{(A-38)}$$

Comparing Eqs (A-38) and (A-31) it is obvious that K^g is defined by

$$K^g R(\hat{r}) = \frac{1}{\sigma_t}\left[R(\hat{r}) + \sum_{\ell,m}\left\{\frac{\sigma_\ell^g}{\sigma_t - \sigma_\ell^g}\right\}\cdot Y_{\ell m}(\hat{r})\int_{4\pi} R(\hat{r}')Y_{\ell m}^*(\hat{r}')d\hat{r}'\right] \qquad \text{(A-39)}$$

a similar derivation for K^u would produce

$$K^u R(\hat{r}) = \frac{1}{\sigma_t}\left[R(\hat{r}) + \sum_{\ell,m}\left\{\frac{\sigma_\ell^u}{\sigma_t - \sigma_\ell^u}\right\}\cdot Y_{\ell m}(\hat{r})\int_{4\pi} Y_{\ell m}^*(\hat{r}')R(\hat{r}')d\hat{r}'\right] \qquad \text{(A-40)}$$

Appendix B

Weak-Form of the Functional

The functional whose Euler equation is the even parity Boltzmann equation of Chapter III is

$$F(u) = \int_R \Big\{ \langle \hat{\Omega}\cdot\nabla u, K^u(\hat{\Omega}\cdot\nabla u) \rangle + \langle u, G^g u \rangle - 2\langle \hat{\Omega}\cdot\nabla u, K^u S^u \rangle$$

$$- 2\langle u, S^g \rangle \Big\} d\bar{r} + \oint_S \Big\{ \int_{4\pi} |\hat{\Omega}\cdot\hat{n}|\, u^2 d\hat{\Omega} \Big\} d\bar{S} \qquad \text{(B-1)}$$

where the inner product <f,g> is defined as

$$\langle f, g \rangle = \int_{4\pi} f^*(\hat{\Omega})\, g(\hat{\Omega})\, d\hat{\Omega} \qquad \text{(B-2)}$$

and * means the complex conjugate.

The minimizing function of this functional is the function Ψ which is a solution to the second order even parity Boltzmann equation (Ref 10:169) Therefore, a solution to the even parity Boltzmann equation can be found by minimizing Eq (B-1).

Another more useful formulation of this problem is the weak form. This weak form can be found by imposing the condition that a function which satisfies the natural boundary conditions Eqs (41) and (42) and the even parity Boltzmann euqation must also be a minimum of the functional (B-1).

Let the functional, (Eq (B-1), have a minimum at Ψ. Then, for all η and ε where ε can be arbitrarily small and of either sign

$$F(\Psi) \leq F(\Psi + \varepsilon\eta) \qquad \text{(B-3)}$$

where Ψ and η are real functions that satisfy the boundary conditions.

Expanding Eq (B-1) in $\Psi+\varepsilon\eta$ gives

$$F(\Psi+\varepsilon\eta) = \int_R \langle \hat{\Omega}\cdot\nabla\Psi, K^u(\hat{\Omega}\cdot\nabla\Psi)\rangle dF \tag{B-4}$$

$$+\varepsilon\int_R \langle \hat{\Omega}\cdot\nabla\Psi, K^u(\hat{\Omega}\cdot\nabla\eta)\rangle dF \tag{B-5}$$

$$+\varepsilon\int_R \langle \hat{\Omega}\cdot\nabla\eta, K^u(\hat{\Omega}\cdot\nabla\Psi)\rangle dF \tag{B-6}$$

$$+\varepsilon^2\int_R \langle \hat{\Omega}\cdot\nabla\eta, K^u(\hat{\Omega}\cdot\nabla\eta)\rangle dF \tag{B-7}$$

$$+\int_R \langle \Psi, G^g\Psi\rangle dF \tag{B-8}$$

$$+\varepsilon\int_R \langle \Psi, G^g\eta\rangle dF \tag{B-9}$$

$$+\varepsilon\int_R \langle \eta, G^g\Psi\rangle dF \tag{B-10}$$

$$+\varepsilon^2\int_R \langle \eta, G^g\eta\rangle dF \tag{B-11}$$

$$-2\int_R \langle \hat{\Omega}\cdot\nabla\Psi, K^u S^u\rangle dF \tag{B-12}$$

$$-2\varepsilon\int_R \langle \hat{\Omega}\cdot\nabla\eta, K^u S^u\rangle dF \tag{B-13}$$

$$-2\int_R \langle \Psi, S^g\rangle dF \tag{B-14}$$

$$-2\varepsilon\int_R \langle \eta, S^g\rangle dF \tag{B-15}$$

$$+\oint_S\int_{4\pi} |\hat{\Omega}\cdot\hat{n}|\,\Psi^2\, d\hat{\Omega}\, d\hat{S} \tag{B-16}$$

$$+2\varepsilon\oint_S\int_{4\pi} |\hat{\Omega}\cdot\hat{n}|\,\Psi\eta\, d\hat{\Omega}\, d\hat{S} \tag{B-17}$$

$$+\varepsilon^2\oint_S\int_{4\pi} |\hat{\Omega}\cdot\hat{n}|\,\eta^2\, d\hat{\Omega}\, d\hat{S} \tag{B-18}$$

noting that (B-4) + (B-8) + (B-12) + (B-14)

+ (B-16) = $F(\Psi)$ (B-19)

and that K^g, K^u, G^g and G^u are self adjoint operators (Ref 10:174), where if L is self adjoint then

$$\begin{aligned}\langle Lf(\hat{\Omega}), g(\hat{\Omega})\rangle &= \langle f(\hat{\Omega}), Lg(\hat{\Omega})\rangle \\ &= \langle Lg(\hat{\Omega}), f(\hat{\Omega})\rangle^* \end{aligned} \tag{B-20}$$

* means the complex congugate. Since η and Ψ are both real functions (B-5) = (B-6) and (B-9) = (B-10). Therefore, collecting terms and simplifying

$$\begin{aligned} F(\Psi+\varepsilon\eta) = F(\Psi) + 2\varepsilon\Big[\int_R \Big\{&\langle \hat{\Omega}\cdot\nabla\eta, K^u(\hat{\Omega}\cdot\nabla\Psi)\rangle \\ &+ \langle \eta, G^g\Psi\rangle - \langle \hat{\Omega}\cdot\nabla\eta, K^u S^u\rangle - \langle \eta, S^g\rangle\Big\} d\hat{r} \\ &+ \oint_S\int_{4\pi} |\hat{\Omega}\cdot\hat{n}|\Psi\eta\, d\hat{\Omega}\, d\hat{s}\Big] + \varepsilon^2\Big[\int_R\Big\{\langle \hat{\Omega}\cdot\nabla\eta, K^u(\hat{\Omega}\cdot\nabla\eta)\rangle \\ &+ \langle \eta, G^g\eta\rangle\Big\} d\hat{r} + \oint_S\int_{4\pi} |\hat{\Omega}\cdot\hat{n}|\eta^2 d\hat{\Omega}\, d\hat{r}\Big] \end{aligned} \tag{B-21}$$

With both K^u and G^g being positive definite operators then the ε^2 term of (B-21) must also be positive. Note that ε^2 is always positive. Now in order to ensure that $F(\Psi+\varepsilon\eta) > F(\Psi)$ for $\varepsilon \neq 0$, the ε term in equation (B-21) must be positive or zero. But ε can be of either sign therefore the coefficient of ε must be zero, that is

$$\begin{aligned} \int_R\Big\{&\langle \hat{\Omega}\cdot\nabla\eta, K^u(\hat{\Omega}\cdot\nabla\Psi)\rangle + \langle \eta, G^g\Psi\rangle - \langle \hat{\Omega}\cdot\nabla\eta, K^u S^u\rangle \\ &- \langle \eta, S^g\rangle\Big\} d\hat{r} + \oint_S\int_{4\pi} |\hat{\Omega}\cdot\hat{n}|\Psi\eta\, d\hat{\Omega}\, d\hat{s} = 0 \end{aligned} \tag{B-22}$$

Eq (B-22) is the weak or Galerkin form of the second order even parity Boltzmann equation. A detailed derivation of equation (B-22) can be found elsewhere (Ref 5:57).

Appendix C

Derivation of the Weak Form From the Galerkin Method of Weighted Residuals

It can be shown that solutions to the second order forms of the Boltzmann equation, by using a variational principle or the method of weighted residuals are equivalent. A proof of this equivalency for the even parity equation is outlined below. However, a similar proof can also be extended to the odd parity second order equation.

The starting point of this proof is the even parity Boltzmann equation

$$-\hat{\Omega}\cdot\nabla K^{u}(\bar{r})\hat{\Omega}\cdot\nabla\psi(\bar{r},\hat{\Omega})+\sigma^{g}(\bar{r})\psi(\bar{r},\hat{\Omega})=S^{g}(\bar{r},\hat{\Omega})-\hat{\Omega}\cdot\nabla K^{u}(\bar{r})S^{u}(\bar{r},\hat{\Omega}) \qquad \text{(C-1)}$$

and vacuum boundary conditions

$$\psi(\bar{r}_s,\hat{\Omega})+K^{u}(\bar{r}_s)\left\{S^{u}(\bar{r}_s,\hat{\Omega})-\hat{\Omega}\cdot\nabla\psi(\bar{r}_s,\hat{\Omega})\right\}=0 \quad \text{for } \hat{\Omega}\cdot\hat{n}<0 \qquad \text{(C-2)}$$

$$\psi(\bar{r}_s,\hat{\Omega})-K^{u}(\bar{r}_s)\left\{S^{u}(\bar{r}_s,\hat{\Omega})-\hat{\Omega}\cdot\nabla\psi(\bar{r}_s,\hat{\Omega})\right\}=0 \quad \text{for } \hat{\Omega}\cdot\hat{n}>0 \qquad \text{(C-3)}$$

In the following equations the $\hat{r}$ and $\hat{\Omega}$ dependences will be omitted.

If a trial solution Ψ is assumed where Ψ is a linear combination of functions such that

$$\Psi=\sum_{i=1}^{N}A_i\psi_i \qquad \text{(C-4)}$$

then the Galerkin method of weighted residuals requires a weight or test function η; where

$$\eta = \sum_{i=1}^{N} \psi_i \qquad \text{(C-5)}$$

The requirement that Ψ should be an exact solution to the problem is imposed by substituting Eq (C-4) into (C-1), and then requiring that the Euclidean norm of the right and left hand sides of (C-1), with respect to the weight function η, are equal.

Applying this requirement to Eq (C-1) gives

$$\int_R \left\{ -\langle \overbrace{\hat{\Omega}\cdot\nabla K^{u}\hat{\Omega}\cdot\nabla\Psi}^{A}, \eta\rangle + \langle G^{g}\Psi, \eta\rangle \right\} dF$$

$$= \int_R \left\{ \langle S^{g}, \eta\rangle - \langle \overbrace{\hat{\Omega}\cdot\nabla K^{u} S^{u}}^{B}, \eta\rangle \right\} dF \qquad \text{(C-6)}$$

where the inner product is defined as

$$\langle f, g\rangle = \int_{4\pi} f^{*} g \, d\hat{\Omega} \qquad \text{(C-7)}$$

and the trial and weight functions, Ψ and η are real functions.

Using the vector identity (Ref 10:169)

$$\int_R \langle \hat{\Omega}\cdot\nabla\eta, f\rangle dF = -\int_R \langle \eta, \hat{\Omega}\cdot\nabla f\rangle dF$$

$$+ \oint_S \langle (\hat{\Omega}\cdot\hat{n})\eta, f\rangle d\hat{s} \qquad \text{(C-8)}$$

terms A and B of Eq (C-6) becomes

$$\int_R -\langle \hat{\Omega}\cdot\nabla K^{u}\hat{\Omega}\cdot\nabla\Psi, \eta\rangle dF = \int_R \langle K^{u}\hat{\Omega}\cdot\nabla\Psi, \hat{\Omega}\cdot\nabla\eta\rangle dF$$

$$-\oint_S \langle (\hat{\Omega}\cdot\hat{n}) K^{u}\hat{\Omega}\cdot\nabla\Psi, \eta\rangle d\hat{s} \qquad \text{(C-9)}$$

$$\int_R -\langle \hat{\Omega}\cdot\nabla K^u S^u; \eta\rangle dF = \int_R \langle K^u S^u; \hat{\Omega}\cdot\nabla\eta\rangle dF$$

$$-\oint_S \langle (\hat{\Omega}\cdot\hat{n}) K^u S^u; \eta\rangle d\bar{s} \qquad \text{(C-10)}$$

Substituting Eq (C-9) and (C-10) into (C-6) gives

$$\int_R \left\{ \langle \hat{\Omega}\cdot\nabla\eta, K^u \hat{\Omega}\cdot\nabla\psi\rangle + \langle G^g \psi, \eta\rangle \right\} dF$$

$$+ \oint_S \left\{ \overset{A}{\langle (\hat{\Omega}\cdot\hat{n}) K^u S^u; \eta\rangle} - \langle (\hat{\Omega}\cdot\hat{n}) K^u \hat{\Omega}\cdot\nabla\psi, \eta\rangle \right\} d\bar{s}$$

$$= \int_R \left\{ \langle \hat{\Omega}\cdot\nabla\eta\rangle, K^u S^u\rangle + \langle \eta, S^g\rangle \right\} dF \qquad \text{(C-11)}$$

term A of Eq (C-11) can be rearranged into

$$A = \oint_S \int_{4\pi} (\hat{\Omega}\cdot\hat{n}) K^u \left\{ S^u - \hat{\Omega}\cdot\nabla\psi \right\} \eta \, d\hat{\Omega} \, d\bar{s} \qquad \text{(C-12)}$$

Using the boundary condition of Eq (C-2) and (C-3), Eq (C-12) can be written as

$$A = \oint_S \left\{ \int_{\hat{\Omega}\cdot\hat{n}>0} (\hat{\Omega}\cdot\hat{n}) \psi \eta \, d\hat{\Omega} - \int_{\hat{\Omega}\cdot\hat{n}<0} (\hat{\Omega}\cdot\hat{n}) \eta \psi \, d\hat{\Omega} \right\} d\bar{s} \qquad \text{(C-13)}$$

Eq (C-12) can also be written as

$$A = \oint_S \int_{4\pi} |\hat{\Omega}\cdot\hat{n}| \psi \eta \, d\hat{\Omega} \, d\hat{s} \qquad \text{(C-14)}$$

where $|\;|$ means the absolute value. Substituting Eq (C-14) into (C-11) gives

$$\int_R \left\{ \langle \hat{\Omega}\cdot\nabla\eta, K^u \hat{\Omega}\cdot\nabla\psi\rangle + \langle G^g \psi, \eta\rangle \right\} dF + \oint_S \int_{4\pi} |\hat{\Omega}\cdot\hat{n}| \psi \eta \, d\hat{\Omega} \, d\hat{s}$$

$$= \int_R \left\{ \langle \hat{\Omega}\cdot\nabla\eta, K^u S^u\rangle + \langle \eta, S^g\rangle \right\} dF \qquad \text{(C-15)}$$

Eq (C-15) is the weak or Galerkin form of the even parity Boltzmann equation. It is identical to Eq (B-22) of Appendix B.

Appendix D

Expansion Properties of Spherical Harmonics

In Chapters III and IV the angular dependence of the trial functions and cross sections was expanded in spherical harmonics. Because of the two dimensional angular dependence in μ and χ, and the requirement that the expansion functions should form a complete set, the expansion is presented with m and ℓ subscripts as follows (Ref 6:608)

$$f(\hat{\Omega}) = \sum_{\ell=0}^{L} \sum_{m=-\ell}^{+\ell} f_{\ell,m} Y_{\ell,m}(\hat{\Omega}) \tag{D-1}$$

or

$$f(\mu,\chi) = \sum_{\ell=0}^{L} \sum_{m=-\ell}^{+\ell} f_{\ell,m} Y_{\ell,m}(\mu,\chi) \tag{D-2}$$

where

$$f_{\ell,m} = \int_0^{2\pi} \int_{-1}^{+1} f(\mu,\chi)\, Y^*_{\ell m}(\mu,\chi)\, d\mu\, d\chi \tag{D-3}$$

and

$$Y_{\ell m}(\mu,\chi) = C_{\ell m} P_{\ell m}(\mu) e^{im\chi} \tag{D-4}$$

and

$$Y_{\ell,-m}(\mu,\chi) = (-1)^m Y^*_{\ell,m}(\mu,\chi) \tag{D-5}$$

and

$$C_{\ell m} = \sqrt{\frac{2\ell+1}{4\pi} \cdot \frac{(\ell-m)!}{(\ell+m)!}} \tag{D-6}$$

If $f(\mu,\chi)$ is even in the angle χ then the expansion must also be even in χ, and therefore, (D-4) can be rewritten as

$$\mathrm{Re}\left[Y_{\ell,m}\right] = Q_{\ell,m} = C_{\ell,m} P_{\ell,m}(\mu) \cos(m\chi) \qquad \text{(D-7)}$$

where the odd $i\sin\chi$ term is omitted. Also from Eq (D-5)

$$Q_{\ell,-m} = (-1)^m C_{\ell,m} P_{\ell,m}(\mu) \cos(m\chi) = (-1)^m Q_{\ell,m} \qquad \text{(D-8)}$$

Therefore for an even expansion Eq (D-3) can be written as

$$f_{\ell,m} = \int_0^{2\pi}\int_{-1}^{+1} f(\mu,\chi) Q_{\ell,m}(\mu,\chi)\, d\mu\, d\chi \qquad \text{(D-9)}$$

and

$$f_{\ell,-m} = \int_0^{2\pi}\int_{-1}^{+1} (-1)^m f(\mu,\chi) Q_{\ell,m}(\mu,\chi)\, d\mu\, d\chi = (-1)^m f_{\ell,m} \qquad \text{(D-10)}$$

For an even χ expansion of $f(\mu,\chi)$ Eq (D-2) can therefore be written as

$$f(\mu,\chi) = \sum_{\ell=0}^{L}\left[f_{\ell 0} Q_{\ell 0} + 2\sum_{m=1}^{\ell} f_{\ell,m} Q_{\ell,m}\right] \qquad \text{(D-11)}$$

or

$$f(\mu,\chi) = \sum_{\ell=0}^{L}\sum_{m=0}^{\ell} f_{\ell,m} Q_{\ell,m} \qquad \text{(D-12)}$$

where the factor of two has been included in the $f_{\ell,m}$ expansion coefficients and Eq (D-12) forms a complete set.

A similar approach can be used for the cross-section expansion

$$\sigma^s(\hat{\Omega}\cdot\hat{\Omega}') = \sum_{\ell=0}^{L} \frac{2\ell+1}{4\pi}\cdot \sigma_\ell^s\, P_\ell(\hat{\Omega}\cdot\hat{\Omega}')$$

$$= \sum_{\ell=0}^{L} \sum_{m=-\ell}^{+\ell} \sigma_\ell^s\, Y_{\ell m}^*(\hat{\Omega}')\, Y_{\ell m}(\hat{\Omega}) \qquad \text{(D-13)}$$

where $P_\ell(\hat{\Omega}\cdot\hat{\Omega}')$ is given by Eq (A-24).

Eq (D-13) can be expanded to give

$$\sigma^s(\hat{\Omega}\cdot\hat{\Omega}') = \sum_{\ell=0}^{L} \Big[\sigma_\ell^s\, Y_{\ell 0}^*(\hat{\Omega}')\, Y_{\ell 0}(\hat{\Omega}) + \sum_{m=1}^{\ell} \sigma_\ell^s\, Y_{\ell m}^*(\hat{\Omega}')\, Y_{\ell m}(\hat{\Omega})$$

$$+ \sum_{m=1}^{\ell} \sigma_\ell^s\, Y_{\ell,-m}^*(\hat{\Omega}')\, Y_{\ell,-m}(\hat{\Omega}) \Big] \qquad \text{(D-14)}$$

and from Eq (D-5)

$$Y_{\ell,m}^*(\hat{\Omega}')\, Y_{\ell,m}(\hat{\Omega}) = Y_{\ell,-m}^*(\hat{\Omega}')\, Y_{\ell,-m}(\hat{\Omega}) \qquad \text{(D-15)}$$

Therefore (D-14) becomes

$$\sigma^s(\hat{\Omega}\cdot\hat{\Omega}') = \sum_{\ell=0}^{L} \Big[\sigma_0^s\, Y_{\ell 0}^*(\hat{\Omega}')\, Y_{\ell 0}(\hat{\Omega}) + 2 \sum_{m=1}^{\ell} \sigma_\ell^s\, Y_{\ell m}^*(\hat{\Omega}')\, Y_{\ell m}(\hat{\Omega}) \Big]$$

$$= 2 \sum_{\ell=0}^{L} \sum_{m^*=0}^{\ell} \sigma_\ell^s\, Y_{\ell m}^*(\hat{\Omega}')\, Y_{\ell m}(\hat{\Omega}) \qquad \text{(D-16)}$$

where m^* means that <u>all terms with a m = 0 subscript must be divided by two</u>.

Since the scattering cross-sections are real the expansion of Eq (D-16) must also be real and with

$$\mathrm{Re}\Big[Y_{\ell m}^*(\hat{\Omega}')\, Y_{\ell m}(\hat{\Omega}) \Big] = C_{\ell m}^2\, P_{\ell m}(\mu')\, P_{\ell m}(\mu) \cos m(\phi-\phi') \qquad \text{(D-17)}$$

Eq (D-16) can be written as

$$\sigma^s(\hat{\Omega}\cdot\hat{\Omega}') = 2 \sum_{\ell=0}^{L} \sum_{m^*=0}^{\ell} \sigma_\ell^s\, C_{\ell m}^2\, P_{\ell m}(\mu')\, P_{\ell m}(\mu) \cos m(\phi-\phi') \qquad \text{(D-18)}$$

Note that

$$\cos m(\chi-\chi') = \cos m\chi \cdot \cos m\chi' + \sin m\chi \cdot \sin m\chi' \qquad \text{(D-19)}$$

The angles μ and χ are shown in Fig. 2.

Similar derivations would give

$$\sigma_s^g(\hat{\Omega}\cdot\hat{\Omega}') = 2\sum_{l=0}^{L}\sum_{m^*=0}^{l} \sigma_l^g C_{lm}^2 P_{lm}(\mu') P_{lm}(\mu) \cos m(\chi-\chi') \qquad \text{(D-20)}$$

and

$$\sigma_s^u(\hat{\Omega}\cdot\hat{\Omega}') = 2\sum_{l=0}^{L}\sum_{m^*=0}^{l} \sigma_l^u C_{lm}^2 P_{lm}(\mu') P_{lm}(\mu) \cos m(\chi-\chi') \qquad \text{(D-21)}$$

By inserting Eq (D-20) into Eq (A-22) the even parity collision operator can now be written as

$$G^g = \left[\sigma_t - 2\sum_{l=0}^{L}\sum_{m^*=0}^{l} \sigma_l^g C_{lm}^2 P_{lm}(\mu) \int_{4\pi} P_{lm}(\mu') \cos m(\chi-\chi')\, d\hat{\Omega}'\right] \qquad \text{(D-22)}$$

and from Eqs (D-15) and (D-17) the inverse odd parity collison operator Eq (A-40), can be written as

$$K^u = \sigma_t^{-1}\left[1 + 2\sum_{l=0}^{L}\sum_{m^*=0}^{l} \left\{\frac{\sigma_l^u}{\sigma_t-\sigma_l^u}\right\} C_{lm}^2 P_{lm}(\mu) \int_{4\pi} P_{lm}(\mu') \cos m(\chi-\chi')\, d\hat{\Omega}'\right] \qquad \text{(D-23)}$$

Similar expression for G^u and K^g can be written.

Some useful properties of spherical harmonics and the associated Legendre functions are (Ref 15: 5:609)

$$P_{l,m}(-\mu) = (-1)^{l-m} P_{l,m}(\mu) \qquad \text{(D-24)}$$

$$P_{\ell,-m}(\mu) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_{\ell m}(\mu) \tag{D-25}$$

$$\int_{-1}^{+1} P_{\ell,m}(\mu) P_{\ell' m}(\mu)\, d\mu = \frac{2}{2\ell+1} \cdot \frac{(\ell+m)!}{(\ell-m)!} \delta_{\ell\ell'} \tag{D-26}$$

where

$$\delta_{\ell\ell'} = \begin{cases} 0 & \text{for } \ell \neq 0 \\ 1 & \text{for } \ell = 0 \end{cases} \tag{D-27}$$

$$\int_0^{2\pi}\int_{-1}^{+1} Y_{\ell m}(\mu,\chi)\, Y^*_{\ell' m'}(\mu, \quad)\, d\mu\, d\chi = \delta_{\ell\ell'}\delta_{mm'} \tag{D-28}$$

Appendix E

The Synthesized Boltzmann Equation

In order to formulate a numerical solution to the air-over-ground problem it is necessary to expand the weak form of the even parity Boltzmann equation in a set of trial and test functions. The finite element space-angle synthesis trial and weight functions of Chapter IV will be used in this expansion. Because this is a very tedious and lengthy derivation, the more obvious albegraic steps will be omitted. The starting point of this formulation is the synthesized even parity Boltzmann equation, Eq (58), of Chapter III.

$$\sum_{iz=1}^{IZ}\sum_{ir=1}^{IR}\sum_{\ell=0}^{L}\sum_{m=0}^{\ell} A_{i,j,\ell,m}\left[\int_R\left\{\langle\hat{\Omega}\cdot\nabla(B_j Q_{kn}), K^u(\hat{\Omega}\cdot\nabla(B_i Q_{\ell m}))\rangle\right.\right.$$

$$\left.+\langle B_j Q_{kn}, G^g(B_i Q_{\ell m})\rangle\right\} d\bar{r} + \oint_S\int_{4\pi}|\hat{\Omega}\cdot\hat{n}| B_j Q_{kn} B_i Q_{\ell m} d\hat{\Omega}\, d\bar{s}$$

$$= \int_R\left\{\langle\hat{\Omega}\cdot\nabla(B_j Q_{kn}), K^u S^u\rangle + \langle B_j Q_{kn}, S^g\rangle\right\} d\bar{r} \qquad \text{(E-1)}$$

where B_i and B_j are tensor products of cubic polynomial splines, and they are given by

$$B_i = B_{iz}(z)\, B_{ir}(\rho) \qquad \text{(E-2)}$$

$$B_j = B_{jz}(z)\, B_{jr}(\rho) \qquad \text{(E-3)}$$

also

$$Q_{\ell m} = C_{\ell m} P_{\ell m}(\mu)\cos m\chi \qquad \text{(E-4)}$$

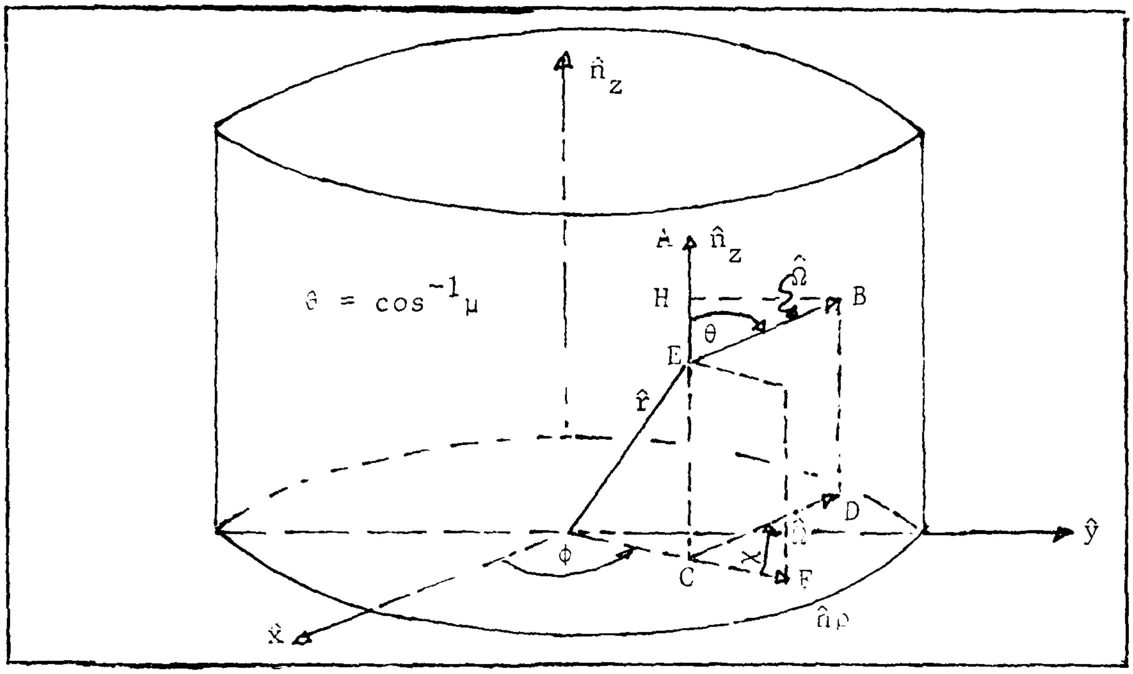

Figure 9. Surface Normal And Particle Velocity Direction Vectors.

and

$$C_{\ell m} = \sqrt{\frac{2\ell+1}{4\pi} \cdot \frac{(\ell-m)!}{(\ell+m)!}} \tag{E-5}$$

$P_{\ell m}(\mu)$ are the associated Legendre functions.

The directional derivative is given as

$$\hat{\Omega} \cdot \nabla\phi = \frac{\alpha}{\rho}\frac{\partial}{\partial\rho}(\rho\phi) - \frac{1}{\rho}\frac{\partial\{\phi\beta(\mu,\chi)\}}{\partial\chi} + \mu\frac{\partial\phi}{\partial z} \tag{E-6}$$

where

$$\alpha = \alpha(\mu,\chi) = \sqrt{1-\mu^2}\cos\chi \tag{E-7}$$

and

$$\beta = \beta(\mu,\chi) = \sqrt{1-\mu^2}\sin\chi \tag{E-8}$$

also

$$\hat{\Omega}\cdot\hat{n} = \begin{cases} \hat{\Omega}\cdot\hat{n}_z & \text{for the horizontal top and bottom surfaces, and} \\ \hat{\Omega}\cdot\hat{n}_\rho & \text{for the vertical (side) of the problem cylinder} \end{cases} \tag{E-9}$$

$\hat{n}_z$ and $\hat{n}_\rho$ are shown in Fig. 7.

If $\hat{\Omega}$, $\hat{n}_r$ and $\hat{n}_z$ are considered to be unit vectors then from Fig. 7

$$AE = EB = CF = 1 \tag{E-10}$$

and therefore for the top surface of the cylinder

$$\hat{\Omega} \cdot \hat{n}_z = AE \times EB \times \cos\theta = \mu \tag{E-11}$$

and for the bottom surface

$$\hat{\Omega} \cdot n_z = -\mu \tag{E-12}$$

also CD = HB = projection of $\hat{\Omega}$ unto the x-y plane and therefore,

$$CD = HB = EB \sin\theta$$

$$= \sqrt{1-\cos^2\theta} = \sqrt{1-\mu^2} \tag{E-13}$$

and

$$\hat{\Omega} \cdot \hat{n}_\rho = CD \times CF \times \cos\chi$$

$$= \sqrt{1-\mu^2}\cos\chi \tag{E-14}$$

In Appendix D the even and odd operators were given as

$$K^u f(\hat{\Omega}) = \sigma_t^{-1}\left[f(\hat{\Omega}) - 2\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\left\{\frac{\sigma_\ell{}^u}{(\sigma_t - \sigma_\ell{}^u)}\right\}\int_{4\pi} T_{\ell m}(\hat{\Omega}')f(\hat{\Omega}')d\hat{\Omega}'\right] \tag{E-15}$$

and

$$G^g f(\hat{\Omega}) = \sigma_t f(\hat{\Omega}) - 2\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma_\ell^g\int_{4\pi} T_{\ell m}(\hat{\Omega}')f(\hat{\Omega}')d\hat{\Omega}' \tag{E-16}$$

where m^* means that all terms with a m = 0 index <u>must be</u> divided by two, and

$$T_{\ell m}(\hat{\Omega}) = C_{\ell m}^2 P_{\ell m}(\mu') P_{\ell m}(\mu) \cos m(\chi - \chi') \qquad \text{(E-17)}$$

Also the inner product is defined as

$$\langle f, g \rangle = \int_{4\pi} f^* g \, d\hat{\Omega}$$

$$= \int_{4\pi} f g \, d\hat{\Omega} \quad \text{for real } f \qquad \text{(E-18)}$$

Using Eqs (E-16), (E-15), (E-14), (E-11), (E-12) and (E-6) and noting that $T_{\ell m}$, $Q_{\ell m}$, B_i and B_j are all real functions, Eq (E-1) can be expanded to give

$$\sum_{IZ=1}^{IZ} \sum_{IR=1}^{IR} \sum_{\ell=0}^{L} \sum_{m=0}^{\ell} A_{ij\ell m} \Bigg[\int_R \sigma_t^{-1} \frac{\partial(\rho B_i)}{\partial \rho} \cdot \frac{\partial(\rho B_j)}{\partial \rho} \frac{1}{\rho^2} dv \int_{4\pi} \alpha^2 Q_{\ell m} Q_{kn} d\hat{\Omega} \qquad \text{(E-19)}$$

$$- \int_R \sigma_t^{-1} \frac{\partial(B_j \rho)}{\partial \rho} \cdot \frac{B_i}{\rho^2} dv \int_{4\pi} \alpha \frac{\partial(\beta Q_{\ell m})}{\partial \chi} Q_{kn} d\hat{\Omega} \qquad \text{(E-20)}$$

$$+ \int_R \sigma_t^{-1} \frac{\partial(\rho B_j)}{\partial \rho} \frac{\partial(B_i)}{\partial Z} \frac{1}{\rho} dv \int_{4\pi} \alpha \mu Q_{\ell m} Q_{kn} d\hat{\Omega} \qquad \text{(E-21)}$$

$$- \int_R \sigma_t^{-1} \frac{1}{\rho} \frac{\partial(\rho B_i)}{\partial \rho} \frac{B_j}{\rho} dv \int_{4\pi} \alpha \frac{\partial(\beta Q_{kn})}{\partial \chi} Q_{\ell m} d\hat{\Omega} \qquad \text{(E-22)}$$

$$+ \int_R \sigma_t^{-1} \frac{1}{\rho^2} B_i B_j \, dv \int_{4\pi} \frac{\partial(\beta Q_{\ell m})}{\partial \chi} \cdot \frac{\partial(\beta Q_{kn})}{\partial \chi} d\hat{\Omega} \qquad \text{(E-23)}$$

$$- \int_R \sigma_t^{-1} \frac{\partial(B_i)}{\partial Z} \frac{B_j}{\rho} dv \int_{4\pi} \mu Q_{\ell m} \cdot \frac{\partial(Q_{kn} \beta)}{\partial \chi} d\hat{\Omega} \qquad \text{(E-24)}$$

$$+\int_R \sigma_t^{-1} \frac{\partial}{\partial \rho}(\rho B_i) \cdot \frac{\partial}{\partial Z}(B_j) \cdot \frac{1}{\rho} dv \int_{4\pi} \mu Q_{kn} \cdot \alpha Q_{\ell m} d\hat{r} \qquad \text{(E-25)}$$

$$-\int_R \sigma_t^{-1} \frac{\partial}{\partial Z}(B_j) \cdot \frac{B_i}{\rho} dv \int_{4\pi} \mu Q_{kn} \cdot \frac{\partial}{\partial \chi}(\beta Q_{\ell m}) d\hat{r} \qquad \text{(E-26)}$$

$$+\int_R \sigma_t^{-1} \frac{\partial}{\partial Z}(B_j) \cdot \frac{\partial}{\partial Z}(B_i) dv \int_{4\pi} \mu Q_{\ell m} \cdot \mu Q_{kn} d\hat{r} \qquad \text{(E-27)}$$

$$+2\sum_{r=0}^{R}\sum_{s'=0}^{r} \left\{ \int_R \sigma_{tr}^{u} \frac{\partial}{\partial \rho}(\rho B_j) \frac{\partial}{\partial \rho}(\rho B_i) \frac{1}{\rho^2} dv \int_{4\pi} \alpha Q_{kn} \left\{ \int_{4\pi} \alpha Q_{\ell m} T_{rs} d\hat{r}' \right\} d\hat{r} \right. \qquad \text{(E-28)}$$

$$-\int_R \sigma_{tr}^{u} \frac{1}{\rho^2} B_i \cdot \frac{\partial}{\partial \rho}(\rho B_j) dv \int_{4\pi} \alpha Q_{kn} \left\{ \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q_{\ell m}) T_{rs} d\hat{r}' \right\} d\hat{r} \qquad \text{(E-29)}$$

$$+\int_R \sigma_{tr}^{u} \frac{\partial}{\partial Z}(B_i) \cdot \frac{\partial}{\partial \rho}(\rho B_j) \frac{1}{\rho} dv \int_{4\pi} \alpha Q_{kn} \left\{ \int_{4\pi} \mu Q_{\ell m} T_{rs} d\hat{r}' \right\} d\hat{r} \qquad \text{(E-30)}$$

$$-\int_R \sigma_{tr}^{u} \frac{1}{\rho^2} B_j \frac{\partial}{\partial \rho}(\rho B_i) dv \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q_{kn}) \left\{ \int_{4\pi} \alpha Q_{\ell m} T_{rs} d\hat{r}' \right\} d\hat{r} \qquad \text{(E-31)}$$

$$+\int_R \sigma_{tr}^{u} \frac{1}{\rho} B_i \cdot \frac{1}{\rho} B_j dv \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q_{kn}) \left\{ \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q_{\ell m}) T_{rs} d\hat{r}' \right\} d\hat{r} \qquad \text{(E-32)}$$

$$-\int_R \sigma_{tr}^{u} \frac{\partial}{\partial Z}(B_i) \left(\frac{B_j}{\rho}\right) dv \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q_{kn}) \left\{ \int_{4\pi} \mu Q_{\ell m} T_{rs} d\hat{r}' \right\} d\hat{r} \qquad \text{(E-33)}$$

$$+\int_R \sigma_{tr}^{u} \frac{\partial}{\partial \rho}(\rho B_i) \cdot \frac{\partial}{\partial Z}(B_j) \frac{1}{\rho} dv \int_{4\pi} \mu Q_{kn} \left\{ \int_{4\pi} \alpha Q_{\ell m} T_{rs} d\hat{r}' \right\} d\hat{r} \qquad \text{(E-34)}$$

$$-\int_R \sigma_{\epsilon r}^{u} \frac{B_i}{\rho} \cdot \frac{\partial}{\partial Z}(B_j)\, dv \int_{4\pi} \mu\, Q_{kn} \left\{ \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q_{\ell m})\, T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \qquad \text{(E-35)}$$

$$+\int_R \sigma_{\epsilon r}^{u} \frac{\partial}{\partial Z}(B_i) \frac{\partial}{\partial Z}(B_j)\, dv \int_{4\pi} \mu\, Q_{kn} \left\{ Q_{\ell m}\, \mu\, T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \qquad \text{(E-36)}$$

$$+\int_R \sigma_{\epsilon} B_j B_i\, dv \int_{4\pi} Q_{kn} Q_{\ell m}\, d\hat{\Omega} \qquad \text{(E-37)}$$

$$-2 \sum_{r=0}^{R} \sum_{s=0}^{r} \int_R \sigma_r^{s} B_j B_i\, dv \int_{4\pi} Q_{kn} \left\{ \int_{4\pi} Q_{\ell m} T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \qquad \text{(E-38)}$$

$$+\oint_S B_i B_j\, ds \int_{4\pi} \left| \mu \text{ OR } \sqrt{1-\mu^2} \cos \chi \right| Q_{kn} Q_{\ell m}\, d\hat{\Omega} \qquad \text{(E-39)}$$

$$= \int_R \sigma_\epsilon^{-1} \frac{1}{\rho} \frac{\partial}{\partial \rho}(\rho B_j)\, dv \int_{4\pi} \alpha\, Q_{kn}\, S^{u}\, d\hat{\Omega} \qquad \text{(E-40)}$$

$$-\int_R \sigma_\epsilon^{-1} \frac{B_j}{\rho}\, dv \int_{4\pi} \frac{\partial}{\partial \chi}(Q_{kn} \beta)\, S^{u}\, d\hat{\Omega} \qquad \text{(E-41)}$$

$$+\int_R \sigma_\epsilon^{-1} \frac{\partial}{\partial Z}(B_j)\, dv \int_{4\pi} \mu\, Q_{kn}\, S^{u}\, d\hat{\Omega} \qquad \text{(E-'2)}$$

$$+2 \sum_{r=0}^{R} \sum_{s=0}^{r} \left\{ \int_R \sigma_{\epsilon r}^{u} \frac{1}{\rho} \frac{\partial}{\partial \rho}(\rho B_j)\, dv \int_{4\pi} \alpha\, Q_{kn} \left\{ \int_{4\pi} S^{u} T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \right. \qquad \text{(E-4)}$$

$$-\int_R \sigma_{\epsilon r}^{u} \frac{B_j}{\rho}\, dv \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q_{kn}) \left\{ \int_{4\pi} S^{u} T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \qquad \text{(E-4)}$$

$$+\int_R \sigma_{tr}^{u} \frac{\partial}{\partial z}(B_j)\,dv \int_{4\pi} \mu\, Q_{kn} \left\{ \int_{4\pi} S^{u}_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \quad \Bigg\} \tag{E-45}$$

$$+\int_R B_j\, dv \int_{4\pi} Q_{kn} S^{g}\, d\hat{\Omega} \tag{E-46}$$

where

$$\sigma_{tr}^{u} = \sigma_t^{-1} \cdot \frac{\sigma_r^{u}}{\sigma_t - \sigma_r^{u}} \tag{E-47}$$

and

$$\int_{4\pi} d\hat{\Omega} = \int_0^{2\pi}\int_{-1}^{1} d\mu\, d\psi \tag{E-48}$$

Eqs (E-19) to (E-36) is an expansion of the first term of Eq (E-1). Eqs (E-37) and (E-38) is an expansion of the second term. Eq (E-39) is an expansion of the third term. Eqs (E-40) to (E-46) is an expansion of the right hand side of Eq (E-1). σ_r^g, σ_t and σ_{tr}^u are functions of z and they must be included in the spatial or dv integrals. In cylindrical geometry with azimuthal symmetry

$$dV = 2\pi r\, dr\, dz \tag{E-49}$$

and $\int ds$ means an integration over the surface of the problem cylinder, Fig. 9.

For the air-over-ground problem with an exponentially varying air density

$$\sigma_t(z) = \sigma_t(o) e^{-z/sh} \tag{E-50}$$

$$\sigma_{tr}^{u}(z) = \sigma_{tr}(o) e^{+z/sh} \tag{E-51}$$

$$\sigma_r^{g}(z) = \sigma_r^{g}(o) e^{-z/sh} \tag{E-52}$$

where $\sigma_t(o)$, $\sigma_r^g(o)$, $\sigma_{tr}^u o)$ are cross-sections of air at sea level.

Z = the height above sea-level

sh = atmospheric scale height ~ 7km

In Eqs (E-19) to (E-46) the integrals are separated in the space and angle variables. These are double integrals in space and angle. However, they can be separated into single integrals of the μ, χ, ρ and z variables.

Appendix F

Angle Integrals of the Synthesized Second Order Boltzmann Equation

An expansion of the even parity Boltzmann equation has produced twenty-eight integral terms (Appendix E). By a further expansion and separation of the integration variables twenty distinct single angle integrals are formed. These angle integrals are dependent on the degree of the spherical harmonic trial function expansion and independent of the problem parameters. They can be evaluated once and thereafter used as a part of the problem input data. In this research project these integrals were numerically integrated for each combination of the ℓ, m, k and n expansion subscripts. They were then stored as a matrix, and selected products were used to produce each of the twenty-eight angle integrals of Eqs (E-19) to (E-46) in Appendix E.

These twenty integrals are

$$\int_0^{2\pi} \cos^2(\chi)\cos(m\chi)\cos(n\chi)\,d\chi \tag{F-1}$$

$$\int_0^{2\pi} \cos(\chi)\,\frac{\partial}{\partial\chi}\{\sin(\chi)\cos(m\chi)\}\cos(n\chi)\,d\chi \tag{F-2}$$

$$\int_0^{2\pi} \cos(\chi)\cos(m\chi)\cos(n\chi)\,d\chi \tag{F-3}$$

$$\int_0^{2\pi} \frac{\partial}{\partial\chi}\{\sin(\chi)\cdot\cos(m\chi)\}\cdot\frac{\partial}{\partial\chi}\{\sin(\chi)\cos(n\chi)\}\,d\chi \tag{F-4}$$

$$\int_0^{2\pi} \cos(m\chi)\cdot\frac{\partial}{\partial\chi}\{\sin(\chi)\cdot\cos(n\chi)\}\,d\chi \tag{F-5}$$

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$$\int_0^{2\pi} \cos(m\chi)\cos(n\chi)\,d\chi \tag{F-6}$$

$$\int_0^{2\pi} \cos(\chi)\cos(n\chi)\sin(m\chi)\,d\chi \tag{F-7}$$

$$\int_0^{2\pi} \cos(n\chi)\cdot\sin(m\chi)\,d\chi \tag{F-8}$$

$$\int_0^{2\pi} \frac{d}{d\chi}\left\{\cos(n\chi)\sin(\chi)\right\}\sin(m\chi)\,d\chi \tag{F-9}$$

$$\int_0^{\pi/2} \cos(\chi)\cos(m\chi)\cos(n\chi)\,d\chi \tag{F-10}$$

$$\int_{\pi/2}^{3\pi/2} \cos(\chi)\cos(m\chi)\cos(n\chi)\,d\chi \tag{F-11}$$

$$\int_{3\pi/2}^{2\pi} \cos(\chi)\cos(m\chi)\cos(n\chi)\,d\chi \tag{F-12}$$

$$\int_0^{1} \mu\, P_{\ell m}(\mu)P_{kn}(\mu)\,d\mu \tag{F-13}$$

$$\int_{-1}^{0} \mu\, P_{\ell m}(\mu)P_{kn}(\mu)\,d\mu \tag{F-14}$$

$$\int_{-1}^{+1} (1-\mu^2)P_{kn}(\mu)P_{\ell m}(\mu)\,d\mu \tag{F-15}$$

$$\int_{-1}^{+1} \sqrt{1-\mu^2}\cdot\mu\cdot P_{\ell m}(\mu)P_{kn}(\mu)\,d\mu \tag{F-16}$$

$$\int_{-1}^{+1} \sqrt{1-\mu^2}\cdot P_{\ell m}(\mu)P_{kn}(\mu)\,d\mu \tag{F-17}$$

$$\int_{-1}^{+1} \mu^2 P_{\ell m}(\mu)P_{kn}(\mu)\,d\mu \tag{F-18}$$

$$\int_{-1}^{+1} \mu P_{\ell m}(\mu) P_{kn}(\mu) d\mu \tag{F-19}$$

$$\int_{-1}^{+1} P_{\ell m}(\mu) P_{kn}(\mu) d\mu \tag{F-20}$$

A numerical evaluation of all twenty integrals was carried out for a third degree spherical harmonic expansion. This evaluation showed that these integrals are equal to zero for many combinations of the ℓm and kn subscripts.

Integrals (F-10) to (F-14) are a part of the surface integral term which has been partitioned into the outward ($\hat{\Omega}\cdot\hat{n} > 0$) and inward ($\hat{\Omega}\cdot\hat{n} < 0$) directions. This partitioning was incorporated into the weak form derivation of Appendix C.

Appendix G

Space Integrals (Bicubic Splines) of the Synthesized Second Order Even Parity Boltzmann Equation

A trial function expansion of the spatial flux dependence, in the weak form of the even parity Boltzmann equation, has been carried out in Appendix E. Bicubic polynomial splines in the ρ and z variables were used to form a tensor product space. These splines are twice continuously differentiable and have non-zero integrals $\int_R B_i(x)B_j(x)dx$ for all $|i-j|\geq 4$. After a separation of the ρ and z variables of integration seventeen distinct integral forms are produced. These integrals, which include the source integrals, must be evaluated over the entire problem domain. The space integrals of Appendix E are selected products of the following seventeen single integrals.

$$\int_0^R \frac{1}{\rho} \cdot \frac{\partial}{\partial \rho}\{\rho B_{jr}(\rho)\} \cdot \frac{\partial}{\partial \rho}\{\rho B_{ir}(\rho)\} d\rho \tag{G-1}$$

$$\int_0^R \frac{\partial}{\partial \rho}\{\rho B_{jr}(\rho)\} \cdot \frac{B_{ir}(\rho)}{\rho} d\rho \tag{G-2}$$

$$\int_0^R \frac{1}{\rho} B_{jr}(\rho) B_{ir}(\rho) d\rho \tag{G-3}$$

$$\int_0^R \frac{\partial}{\partial \rho}\{\rho B_{jr}(\rho)\} \cdot \frac{B_{ir}(\rho)}{\rho} d\rho \tag{G-4}$$

$$\int_0^R B_{jr}(\rho) \cdot B_{ir}(\rho) d\rho \tag{G-5}$$

$$\int_0^R B_{jr}(\rho) \cdot B_{ir}(\rho) d\rho \tag{G-6}$$

$$\int_0^H e^{z/sh} B_{jz}(z) B_{iz}(z) dz \tag{G-7}$$

$$\int_0^H e^{z/sh} \frac{\partial}{\partial z}\{B_{iz}(z)\} \cdot B_{jz}(z)\, dz \tag{G-8}$$

$$\int_0^H \frac{\partial}{\partial z}\{B_{jz}(z)\} \cdot \frac{\partial}{\partial z}\{B_{iz}(z)\} e^{z/sh}\, dz \tag{G-9}$$

$$\int_0^H B_{iz}(z) \cdot B_{jz}(z) e^{-z/sh}\, dz \tag{G-10}$$

$$\int_0^H B_{iz}(z) \cdot B_j(z)\, dz \tag{G-11}$$

The Source Integrals

$$\int_0^R \frac{\partial}{\partial \rho}\{\rho B_{jr}(\rho)\} H_j(\rho)\, d\rho \tag{G-12}$$

$$\int_0^R B_{jr}(\rho) \cdot H_j(\rho)\, d\rho \tag{G-13}$$

$$\int_0^R B_{jr}(\rho) H_j(\rho) \rho\, d\rho \tag{G-14}$$

$$\int_0^H B_{jz}(z) H_i(z) e^{z/sh}\, dz \tag{G-15}$$

$$\int_0^H \frac{\partial}{\partial z}\{B_{jz}(z)\} H_i(z) e^{z/sh}\, dz \tag{G-16}$$

$$\int_0^H B_{jz}(z) \cdot H_i(z)\, dz \tag{G-17}$$

where

B(z) = cubic polynomial z-spline

B(x) = cubic polynomial ρ-spline

sh = atmospheric scale height

R = outer radius of the problem cylinder

H = problem cylinder height

$H(z)$ and $H(\rho)$ are the source interpolating functions (linear Lagrange polynomials).

Appendix H

An Expansion of the First Scatter Source in Legendre Polynomials

In Chapter IV the first scatter source was defined as

$$S(\rho, z, \hat{\Omega}) = \sigma^s(z, \hat{\Omega}\cdot\hat{\Omega}')\, \phi_d(\rho, z, \hat{\Omega}') \qquad \text{(H-1)}$$

where

$\phi_d(\hat{r}, z, \hat{\Omega}')$ = direct fluence of Chapter IV, Eq (74)

$\sigma^s(z, \hat{\Omega}\cdot\hat{\Omega}')$ = scattering cross-section

The usual Legendre polynomial cross-section expansion will now be carried out. Also the even and odd parity first scatter source expressions of Chapter IV will be derived. Expanding σ^s in Legendre polynomials and using the addition theorem (see Appendix D)

$$\sigma^s(z, \hat{\Omega}\cdot\hat{\Omega}') = 2\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell} \sigma_\ell^s(z)\, P_{\ell m}(\mu')\, P_{\ell m}(\mu) \cos(m(\chi-\chi')) \qquad \text{(H-2)}$$

where m^* means that all terms with a m = 0 subscript must be divided by two, and

$$\sigma_\ell^s(z) = \sigma_\ell^s(0)\, e^{-z/sh} \qquad \text{(H-3)}$$

From Fig. 5 and Fig. 2 it is apparent that $\mu' = \mu d$ and $\chi' = 0$

Therefore

$$S(\rho,z,\hat{\Omega}) = 2\,\Phi_d(\rho,z,\hat{\Omega}')\,e^{-z/sh} \times \sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell} \sigma_\ell^s(0)\,C_{\ell m}^2\,P_{\ell m}(\mu d)\,P_{\ell m}(\mu)\cos m\chi \quad \text{(H-4)}$$

and using the identity (Ref 18:96)

$$P_{\ell,m}(-\mu) = (-1)^{\ell-m} P_{\ell m}(\mu) \quad \text{(H-5)}$$

and a little algebra, the even and odd parity first scatter sources can be written as

$$S^u(\rho,z,\hat{\Omega}) = \frac{1}{2}\left[S(\rho,z,\hat{\Omega}) - S(\rho,z,-\hat{\Omega})\right]$$
$$= \Phi_d(\rho,z,\hat{\Omega}')e^{-z/sh}\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma_\ell^s(0)C_{\ell m}^2\left[1 - (-1)^{\ell-m}\right]P_{\ell m}(\mu)P_{\ell m}(\mu d)\cos(m\chi) \quad \text{(H-6)}$$

and

$$S^g(\rho,z,\hat{\Omega}) = \frac{1}{2}\left[S(\rho,z,\hat{\Omega}) + S(\rho,z,-\hat{\Omega})\right]$$
$$= \Phi_d(\rho,z,\hat{\Omega}')e^{-z/sh}\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma_\ell^s(0)C_{\ell m}^2\left[1 + (-1)^{\ell-m}\right]P_{\ell m}(\mu)P_{\ell m}(\mu d)\cos(m\chi) \quad \text{(H-7)}$$

Appendix I

A Derivation of the Total Particle Fluence

In Chapter IV a trial function expansion of the even parity angular particle fluence was given as

$$\Psi(\rho,z,\mu,\chi)=\sum_{iz=1}^{IZ}\sum_{ir=1}^{IR}\sum_{\ell=0}^{L}\sum_{m=0}^{\ell} A_{i,j,\ell,m}\, B_{iz}(z)\, B_{ir}(\rho)\, Q_{\ell m} \tag{I-1}$$

where

$$Q_{\ell m} = C_{\ell m} P_{\ell m}(\mu) \cos m\chi \tag{I-2}$$

and

$$C_{\ell m} = \sqrt{\frac{2\ell+1}{4\pi}\cdot\frac{(\ell-m)!}{(\ell+m)!}} \tag{I-3}$$

The $A_{i,j,\ell,m}$ mixing coefficients are obtained from a numerical solution of the second order synthesized Boltzmann equation of Chapter IV.

The angular even parity fluence is also defined as

$$\Psi(\rho,z,\mu,\chi) = \frac{1}{2}\left[\phi(\rho,z,\mu,\chi) + \phi(\rho,z,-\mu,-\chi)\right] \tag{I-4}$$

An integration of Eq (I-4) over all directions gives the total even parity particle fluence $\Psi(\rho,z)$, and also the total particle fluence $\phi(\rho,z)$. This is because

$$\int_{4\pi} \Psi(\rho,z,\mu,\chi)\, d\hat{\Omega} = \Psi(\rho,z) \tag{I-5}$$

$$= \frac{1}{2}\int_{4\pi}\phi(\rho,z,\mu,\chi)\,d\hat{\Omega} + \frac{1}{2}\int_{4\pi}\phi(\rho,z,-\mu,-\chi)\,d\hat{\Omega}$$

$$= \int_{4\pi}\phi(\rho,z,\mu,\chi)\,d\hat{\Omega} = \phi(\rho,z)$$

Therefore

$$\psi(\rho,z) = \phi(\rho,z) \qquad \text{(I-6)}$$

Eq (I-1) will now be integrated to give the total particle fluence at position (ρ,z). Using the orthogonal properties of Legendre polynomials this integration is carried out as follows.

The zero order associated Legendre function is defined as

$$P_{0,0}(\mu) = 1 \qquad \text{(I-7)}$$

Multiplying Eq (I-1) by Eq (I-7) and integrating over all μ and χ directions gives

$$\int_0^{2\pi}\int_{-1}^{1}\psi(\rho,z,\mu,\chi)\,P_{0,0}(\mu)\,d\mu\,d\chi$$

$$= \psi(\rho,z) = \sum_{iz=1}^{IZ}\sum_{ir}^{IR}\sum_{\ell=0}^{L}\sum_{m=0}^{\ell} A_{i,j,\ell,m}\,B_{iz}(z)\,B_{ir}(\rho)$$

$$\times \int_0^{2\pi}\int_{-1}^{+1} Q_{\ell m}\,P_{00}(\mu)\,d\mu\,d\chi \qquad \text{(I-8)}$$

Substituting Eq (I-2) for $Q_{\ell m}$, the integral of Eq (I-8) becomes

$$\int_0^{2\pi}\cos(m\chi)\,d\chi \cdot \int_{-1}^{1} C_{\ell m}\,P_{\ell m}(\mu)\,P_{0,0}(\mu)\,d\mu \qquad \text{(I-9)}$$

where

$$\int_0^{2\pi} \cos(m\chi)\,d\chi = \begin{cases} 0 & \text{for } m \neq 0 \\ 2\pi & \text{for } m = 0 \end{cases} \quad \text{(I-10)}$$

and (see Appendix D)

$$\int_{-1}^{1} C_{\ell,0} P_{\ell,0}(\mu) P_{0,0}(\mu)\,d\mu = \frac{2}{2\ell+1} \cdot \frac{(\ell+0)!}{(\ell-0)!} \delta_{\ell 0} \cdot C_{\ell 0}$$

$$= 2C_{0,0} = 2/\sqrt{4\pi} \quad \text{(I-11)}$$

therefore Eq (I-9) becomes

$$2\pi \cdot 2/\sqrt{4\pi} = \sqrt{4\pi} \quad \text{(I-12)}$$

and the total particle fluence is

$$\phi(\rho,z) = \psi(\rho,z) = \sqrt{4\pi} \sum_{iz=1}^{IZ} \sum_{ir=1}^{IR} A_{ij\ell m} B_{iz}(z) B_{ir}(\rho) \quad \text{(I-13)}$$

where $\ell = m = 0$

The angular particle fluence is given by

$$\phi(\rho,z,\hat{\Omega}) = \psi(\rho,z,\hat{\Omega}) + \chi(\rho,z,\hat{\Omega}) \quad \text{(I-14)}$$

where $\chi(\rho,z,\hat{\Omega})$ is the odd parity fluence, which, is defined in terms of the even parity fluence and source by the following expression

$$\chi(\rho,z,\hat{\Omega}) = K^{u}(\rho)\left[S^{u}(\rho,z,\hat{\Omega}) - \hat{\Omega}\cdot\nabla\psi(\rho,z,\hat{\Omega})\right] \quad \text{(I-15)}$$

Therefore once $\Psi(\rho,z,\hat{\Omega})$ has been found the odd parity fluence and the angular particle fluence $\phi(\rho,z,\hat{\Omega})$ can be computed from Eqs (I-15) and (I-14).

Appendix J

Computer Subroutines

A computer program has been written to solve the synthesized Boltzmann equation of Chapter IV. This program is designed to use a trial function expansion in bicubic splines and spherical harmonics, and to perform a first scatter source interpolation using linear Lagrange polynomials. The program in an assemblage of several subroutines which collectively perform the following tasks.

1. Computes all single space and angle integrals.
2. Combines the single μ and χ angle integrals for all combinations of the spherical harmonic expansion subscripts.
3. Combines the single ρ and z integrals for all combinations of the bicubic spline expansion subscripts.
4. Assembles the coefficient problem matrix.
5. Computes and interpolates the first scatter source.
6. Assembles the source vector.
7. Checks for symmetry and diagonal dominance.
8. Solves for the $A_{i,j,\ell,m}$ expansion (mixing) coefficients by the method of successive over-relaxation.
9. Solves for the total particle fluence.

A ten point Newton-Cotes single integration routine was used to numerically integrate the thirty-seven integrals of Appendices F and G. This integration routine is an in-hou subroutine of the Air Force Aeronautical Systems Division, Wright-Patterson Air Force Base. The overall program logic

has been written in a manner whereby this integration routine could be used. The program is written in Fortran V.

<u>Listing of Problem Subroutines</u>

```
 PROGRAM MAIN
 DIMENSION CL(0:3,0:3),SH(0:3,0:3,12),DUSH(0:3,0:3),PL(3,3,8),DUPL(
13,3),CA(3,3,30),MA(50),C(50)
 DIMENSION PNZ(-2:7),PNR(-2:7),PNX(-2:7),SPZ(7,7,5),SPR(7,7,6),SPX(
17,7,6),XSEVL(0:4),SVZ(7,5,3),SVX(7,5,3),SVR(7,5,3),APD(5,5,3),SB(5
10),AC(50,50),XSODL(0:4),XS(0:4)
 COMMON/A1/PNX,I/A2/ASH//ITYPE,ITS,ITTY
 COMMON/B2/ISH/B3/IP
 ****************************************************************
 * THIS ROUTINE SOLVES THE EVEN PARITY ANISOTROPIC BOLTZMANN      *
 * EQUATION AND THE AIR-OVER GROUND PROBLEM FOR THE REACTION      *
 * RATE FLUENCE BY CALLING A NUMBER OF SUBROUTINES AND USING A    *
 * TEN POINT NEWTON COTES INTEGRATION ROUTINE.
 ****************************************************************
 READ(*,*,END=120)DZ,Z2,R2,DR,Z1,R1,ASH,LMAX
 READ(*,*,END=120)YD,HB,SIGT,W
 PRINT*,'PROBLEM INPUT DATA'
 PRINT*,' '
 PRINT*,'DZ= ',DZ,'     DR=',DR,'     R2=',R2,'      Z2=',Z2,'      ASH=
1,ASH,'     Z1=',Z1,'     R1=',R1,' RELAXATION FACTOR =',W
 PRINT*,' '
 PRINT*,' LEGENDRE EXPANSION P(LMAX)=',LMAX
 READ(*,*,END=120)(XSEVL(I),I=0,LMAX)
 READ(*,*,END=120)(XSODL(I),I=0,LMAX)
 READ(*,*,END=120)(XS(I),I=0,LMAX)
 PRINT*,'YD=',YD,'    HB=',HB,'      SIGT=',SIGT
 PRINT*,' '
 PRINT*,' LEGENDRE ODD EXPANSION SCATTERING CROSS SECTION. ALL ODD
1MOMENTS ARE ZERO.'
 PRINT*,' '
 PRINT*,('     ',XSEVL(I),I=0,LMAX)
 PRINT*,
 PRINT*,   LEGENDRE ODD PARITY EXPANSION SCATTERING CROSS-SECTION.-
1LL (L) EVEN MOMENTS ARE ZERO.'
 PRINT*,' '
 PRINT*,('     ',XSODL(I),I=0,LMAX)
 PRINT*,' '
 PRINT*,  LEGENDRE EXPANSION CROSS SECTION (ODD AND EVEN).'
 PRINT*,
 PRINT*,(       ,XS(I),I=0,LMAX)
 PRINT*,
 PRINT*,
 IT=(LMAX+1)*(LMAX+2)/2
 ITTY=0
 TOL=.0001
 KOUNT=200
 CALL COEFF(LMAX,CL
```

```
PRINT*,'THE SPHERICAL HARMONIC COEFFICIENTS (L,M) .'
PRINT*,' '
DO 5 L=0,LMAX
PRINT*,('      ',CL(L,M),M=0,L)
PRINT*,' '
PRINT*,' '
X1=0.
X2=8*ATAN(1.)
TOL=.00001
KOUNT=200
ITYPE=1
PRINT*,'  ANGULAR INTEGRALS OF SPHERICAL HARMONICS FOR THE '
PRINT*,'   GALERKIN SOLUTION TO THE EVEN-PARITY FORM OF THE '
PRINT*,'  NEUTRON TRANSPORT EQUATION.'
PRINT*,'  THESE ARE INTEGRALS OVER 2*PHI OF THE REAL AND/OF EVEN
PRINT*,'  PART OF EXP(-IMX), EXPANDED IN SINES AND COSINES.'
PRINT*,' '
DO 15 ISH=1,12
CALL SPHER(LMAX,SH(0,0,ISH),X1,X2,TOL,KOUNT)
PRINT*,'  ANGULAR (HARMONIC) INTEGRAL=',ISH
DO 10 M=0,LMAX
PRINT*,('      ',SH(M,N,ISH),N=0,LMAX)
PRINT*,' '
PRINT*,' '
CONTINUE
X1=-1.0
X2=1.0
ITYPE=2
PRINT*,' THE ASSOCIATED LENGENDRE POLYNOMIALS INTEGRALS FOR THE
PRINT*,'GALERKIN SOLUTION.'
PRINT*,' THESE ARE THE POLYNOMIALS PL(L,M) (ASSOC. LEGENDRE)
PRINT*,' INTEGRATED OVER THE INTERVAL (-1,+1).'
PRINT*,' '
DO 25 IP=1,8
CALL POLY(LMAX,PL(1,1,IP),X1,X2,TOL,KOUNT)
PRINT*,' ASSOCIATED LEGENDRE POLYNOMIAL INTEGRAL=',IP
DO 20 IM=1,KT
PRINT*,('      ',PL(IM,IT,IP),IT=1,KT)
PRINT*,
PRINT*,
CONTINUE
CALL ANGLE(LMAX,CL,SH,PL,CA,SIGT,XSEVL,XSODL,KT,XS)
ITTY=1
NX=(Z2-Z1)/DZ+1.1
DO 30 I=0,NX+2
PNW(I)=Z1+I*DZ
[illegible]
[illegible]
ITYPE=1
[illegible]
PRINT*,'   [illegible] VALUES FOR [illegible] INTEGRALS
PRINT*,
DO 50 I=1,5
CALL [illegible](IST,NST,TOL,KOUNT)
CONTINUE
```

```
ITS=1
PRINT*,'  MATRIX VALUES FOR Z-SPACE SOURCE INTEGRALS'
PRINT*,' '
DO 59 I=1,3
CALL SOURCE(SVZ,NZS,TOL,KOUNT)
CONTINUE
NX=(R2-R1)/DR+1.1
DO 60 I=0,NX+2
RNX(I)=R1+I*DR
IF(RNX(I).EQ.0.0)RNX(I)=1.0E-9
RNR(I)=RNX(I)
NRS=NX+2
NT=KT+KT*((NZS-1)+NZS*(NRS-1))
PRINT*,' '
PRINT*,' '
PRINT*,'  THE TOTAL NUMBER OF TRIAL FUNCTIONS = ',NT
PRINT*,' THE NUMBER OF LEGENDRE FUNCTIONS = ',KT
PRINT*,' '
PRINT*,' '
PRINT*,'  PROBLEM GEOMETRY INPUT DATA.'
PRINT*,'  NODE(Z,R)        MESH COORDINATE(Z,R)'
PRINT*,' '
DO 65 MR=0,NZS-3
DO 65 MC=0,NRS-3
PRINT*,'(',MR,',',MC,')','          ',RNZ(MR),'    ',RNR(MC)
PRINT*,
PRINT*,' '
ITYPE=2
ITS=0
PRINT*,'  MATRIX VALUES FOR R-SPACE INTEGRALS.'
PRINT*,'
DO 90 I=1,6
CALL SPLINE(SRR,NRS,TOL,KOUNT)
CONTINUE
ITS=2
PRINT*,'  MATRIX VALUES FOR R-SPACE SOURCE INTEGRALS.'
PRINT*,
DO 100 I=1,3
CALL SOURCES(SVR,NRS,TOL,KOUNT)
CONTINUE
TO COMPUTE THE INTERPOLATION POINT VALUES
CALL DIRECT(LMAX,APD,RNZ,RNR,NRS,NZS,SIGT,HB,YD,ASH)
TO COMPUTE THE PROBLEM SOURCE VECTOR
CALL BVEC(APD,SVZ,SVR,SB,NZS,NRS,LMAX,CA,SIGT,KT,NT)
TO COMPUTE THE STIFFNESS ATRIX.
CALL STIFF(CA,SRR,SRZ,NZS,NRS,SIGT,AS,RNR,RNZ,LMAX,NT)
TO CHECK THE STIFNESS MATRIX
CALL CHECK(AS,NT)
TO SOLVE THE PROBLEM MATRIX.
CALL SOLVE(N,SB,AS,NT,...)
TO COMPUTE THE SPATIAL SCALAR FLUX AT THE NODES.
PRINT*,
PRINT*,  THE TOTAL SPACIAL SCATTERED AND DIRECT FLUX.
PRINT*,    SPACE POINT Z,R         TOTAL SCATTERED FLUX          TOTA
L DIRECT FLUX         TOTAL FLUX (DIRECT+SCATTERED)
```

```
      MZ=(NZS-3)*2
      MR=(NRS-3)*2
      DZ=(Z2-Z1)/MZ
      DR=(R2-R1)/MR
      DO 110 I=0,MZ
      DO 110 J=0,MR
      R=R1+J*DR
      IF(R.LT.PNR(0))R=PNR(0)
      Z=Z1+I*DZ
      CALL TFLUX(PNR,PNZ,XB,R,Z,KT,NZS,NRS,TPHI,DPHI,HB,SIGT,AIH,YD)
      TFHI=DPHI+TPHI
      PRINT*,' '
      PRINT*,'(',Z,',',R,')','                       ',TPHI,'                 ',DPHI,
     1'      ',TFHI
      CONTINUE
      GO TO 130
      PRINT*,'PREMATURE PROBLEM DATA END'
      STOP
      END
      SUBROUTINE SPHER(LMAX,DUSH,X1,X2,TOL,KOUNT)
      DIMENSION DUSH(0:3,0:3)
      COMMON/B1/M,N/B2/ISH//ITYPE,ITS,ITTY
*****************************************************************
* THIS ROUTINE NUMERICALLY INTEGRATES THE SINES AND COSINES SINGLE
* INTEGRALS OF THE ANISOTROPIC EVEN PARITY BOLTZMANN EQUATION BY *
* USE OF A TEN POINT NEWTON-COTES INTEGRATION ROUTINE.          *
*****************************************************************
      IF(ISH.LE.9)GO TO 20
      IF (ISH.EQ.10) THEN
      X1=0.
      X2=2.*ATAN(1.)
      GO TO 20
      ELSE IF (ISH.EQ.11) THEN
      X2=2.*ATAN(1.)
      X1=6*ATAN(1.)
      GO TO 20
      ELSE IF (ISH.EQ.12) THEN
      X1=6*ATAN(1.)
      X2=8*ATAN(1.)
      ENDIF
      CONTINUE
      DO 30 M=0,LMAX
      DO 30 N=0,LMAX
      CALL QUAD(X1,X2,TOL,DUSH(M,N),KOUNT)
      IF(DUSH(M,N).LT.1.0E-10)DUSH(M,N)=0.
      CONTINUE
      RETURN
      END
      SUBROUTINE POLY(LMAX,DVAL,X1,X2,TOL,KOUNT)
      DIMENSION DVAL(0:3)
      COMMON/B1/M,N/B2/ISH/B4/L,K//ITYPE,ITS,ITTY
*****************************************************************
* THIS ROUTINE COMPUTES THE INTEGRALS OF THE ASSOCIATED LEGENDRE *
* POLYNOMIALS WHICH ARE A PART OF THE SYNTHESIZED EVEN PARITY   *
* BOLTZMANN EQUATION.A TEN POINT NEWTON-COTES INTEGRATION IS
*****************************************************************
```

```
IF(IP.LE.6)GO TO 30
IF (IP.EQ.7) THEN
X1=0.
X2=1.0
GO TO 30
ELSE IF (IP.EQ.8) THEN
X1=0.0
X2=-1.0
ENDIF
CONTINUE
IW=0
DO 40 K=0,LMAX
DO 40 N=0,K
IT=0
IW=IW+1
DO 40 L=0,LMAX
DO 40 M=0,L
IT=IT+1
CALL QUAD(X1,X2,TOL,DUPL(IW,IT),KOUNT)
IF(DUPL(IW,IT).LT.1.0E-10)DUPL(IW,IT)=0.
CONTINUE
RETURN
END
FUNCTION Y(X)
DIMENSION RNX(-2:7)
COMMON /B1/ M,N/B2/ISH/B3/IP/B4/L,K//ITYPE,ITS,ITTY
COMMON /A1/ RNX,I/A2/AIH/A3/JR,JT/A4/KS,IH,LR
******************************************************************
* THIS FUNCTION IS USED BY THE TEN POINT NEWTON COTES INTEGRATION*
* ROUTINE (QUAD) TO SELECT THE INTEGRATION FUNCTIONS.IT USES THE *
* INFORMATION IN THE ABOVE COMMON BLOCKS TO DETERMINE THE FUNCTION
* WHICH IS BEING INTEGRATED.
******************************************************************
IF(ITTY.EQ.1)GO TO 25
IF(ITYPE.EQ.2)GO TO 20
IF (ISH.EQ.1) THEN
Y=COS(X)**2*COS(M*X)*COS(N*X)
RETURN
ELSE IF (ISH.EQ.2) THEN
[illegible]
RETURN
ELSE IF (ISH.EQ.3.OR.ISH.EQ.10.OR.ISH.EQ.11.OR.ISH.EQ.12) THEN
Y=COS(X)*COS(M*X)*COS(N*X)
RETURN
ELSE IF (ISH.EQ.4) THEN
[illegible]
[illegible]
RETURN
[illegible]
[illegible]
RETURN
[illegible]
Y=COS(M*X)*COS(N*X)
RETURN
[illegible]
```

```
Y=COS(X)*COS(N*X)*SIN(M*X)
RETURN
ELSE IF (ISH.EQ.8) THEN
Y=COS(N*X)*SIN(M*X)
RETURN
ELSE IF (ISH.EQ.9) THEN
Y=(COS(X)*COS(N*X)-N*SIN(X)*SIN(N*X))*SIN(M*X)
ENDIF
RETURN
CONTINUE
A=1-X**2
IF(A.LE.1.0E-10)A=0.
IF (IP.EQ.1) THEN
Y=A*PLF(X,K,N)*PLF(X,L,M)
RETURN
ELSE IF (IP.EQ.2) THEN
Y=SQRT(A)*X*PLF(X,K,N)*PLF(X,L,M)
RETURN
ELSE IF (IP.EQ.3) THEN
Y=SQRT(A)*PLF(X,K,N)*PLF(X,L,M)
RETURN
ELSE IF (IP.EQ.4) THEN
Y=X**2*PLF(X,K,N)*PLF(X,L,M)
RETURN
ELSE IF (IP.EQ.5.OR.IP.EQ.7.OR.IP.EQ.8) THEN
Y=X*PLF(X,K,N)*PLF(X,L,M)
RETURN
ELSE IF (IP.EQ.6) THEN
Y=PLF(X,K,N)*PLF(X,L,M)
ENDIF
RETURN
CONTINUE
IF(ITYPE.EQ.2)GO TO 30
IF(ITS.EQ.1)GO TO 120
IF (I.EQ.1) THEN
M=1
N=1
GO TO 70
ELSE IF (I.EQ.2) THEN
M=1
N=2
GO TO 70
ELSE IF (I.EQ.3) THEN
M=2
N=2
GO TO 70
ELSE IF (I.EQ.4) THEN
M=1
N=1
GO TO 70
ELSE IF (I.EQ.5) THEN
M=1
N=1
GO TO 70
ENDIF
CONTINUE
```

```
IF(ITS.EQ.2)GO TO 130
IF (I.EQ.1) THEN
M=3
N=3
GO TO 70
ELSE IF (I.EQ.2) THEN
M=3
N=1
GO TO 70
ELSE IF (I.EQ.3) THEN
M=1
N=1
GO TO 70
ELSE IF (I.EQ.4) THEN
M=3
N=1
GO TO 70
ELSE IF (I.EQ.5) THEN
M=1
N=1
GO TO 70
ELSE IF (I.EQ.6) THEN
M=1
N=1
ENDIF
SP1=SPF(M,K,PNX(JR-3),PNX(JR-2),PNX(JR-1),PNX(JR),X)
SP2=SPF(N,K-JT,PNX(JR+JT-3),PNX(JR+JT-2),PNX(JR+JT-1),PNX(JR+JT),X
1)
IF(ITYPE.EQ.2)GO TO 100
IF (I.LE.3) THEN
Y=EXP(X/ASH)*SP1*SP2
RETURN
ELSE IF (I.EQ.4) THEN
Y=EXP(-X/ASH)*SP1*SP2
RETURN
ELSE IF (I.EQ.5) THEN
Y=SP1*SP2
RETURN
ENDIF
CONTINUE
IF (I.LE.3) THEN
IF(X.EQ.0.)X=1.0E-30
Y=SP1*SP2/X
RETURN
ELSE IF (I.EQ.4.OR.I.EQ.5) THEN
Y=SP1*SP2
RETURN
ELSE IF (I.EQ.6) THEN
Y=SP1*SP2*[illegible]
RETURN
ENDIF
CONTINUE
IF (I.EQ.1) THEN
N=[illegible]
GO TO [illegible]
ELSE IF [illegible] THEN
```

```
N=2
GO TO 140
ELSE IF (I.EQ.3) THEN
N=1
GO TO 140
ENDIF
CONTINUE
IF (I.EQ.1) THEN
N=3
GO TO 140
ELSE IF (I.EQ.2.OR.I.EQ.3) THEN
N=1
ENDIF
SPH1=SPF(N,KS,PNX(LR-3),PNX(LR-2),PNX(LR-1),PNX(LR),X)
SPH2=HIF(IH,PNX(L),PNX(L+1),X)
IF(ITS.EQ.2)GO TO 160
IF (I.EQ.1.OR.I.EQ.2) THEN
Y=SPH1*SPH2*EXP(X/ASH)
RETURN
ELSE IF (I.EQ.3) THEN
Y=SPH1*SPH2
RETURN
ENDIF
CONTINUE
IF (I.EQ.1.OR.I.EQ.2) THEN
Y=SPH1*SPH2
RETURN
ELSE IF (I.EQ.3) THEN
Y=SPH1*SPH2*X
ENDIF
RETURN
END
FUNCTION PLF(X,I,J)
*****************************************************************
* THIS ROUTINE SELECTS AND COMPUTES THE ASSOCIATED LEGENDRE      *
* FUNCTION WHICH IS BEING INTEGRATED.
*****************************************************************
A=1.-X**2
IF(A.LE.1.0E-10)A=0.
B=X**2-1.
IF (I.EQ.0.AND.J.EQ.0) THEN
PLF=1.0
RETURN
ELSE IF (I.EQ.1.AND.J.EQ.0) THEN
PLF=X
RETURN
ELSE IF (I.EQ.1.AND.J.EQ.1) THEN
PLF=-SQRT(A)
RETURN
ELSE IF (I.EQ.2.AND.J.EQ.0) THEN
PLF=[illegible]
RETURN
ELSE IF (I.EQ.2.AND.J.EQ.1) THEN
PLF=[illegible]SQRT(A)
RETURN
ELSE IF (I.EQ.2.AND.J.EQ.2) THEN
```

```
PLF=3*A
RETURN
ELSE IF (I.EQ.3.AND.J.EQ.0) THEN
PLF=(48.*(X**3)+72.*X*B)/48.
RETURN
ELSE IF (I.EQ.3.AND.J.EQ.1) THEN
PLF=-(SQRT(A)*(288*X**2+72*B))/48
RETURN
ELSE IF (I.EQ.3.AND.J.EQ.2) THEN
PLF=15.*X*A
RETURN
ELSE IF (I.EQ.3.AND.J.EQ.3) THEN
PLF=-15.*(A**1.5)
ENDIF
RETURN
END
SUBROUTINE ANGLE(LMAX,CL,SH,PL,CA,SIGT,XSEVL,XSODL,KT,XS)
DIMENSION CL(0:3,0:3),SH(0:3,0:3,12),PL(3,3,8),CA(3,3,30),XSEVL(0:
14),XSODL(0:4),XS(0:4)
:*************************************************************
* THIS ROUTINE ASSEMBLES THE TOTAL ANGLE INTEGRALS FOR ALL
* COMBINATIONS OF THE SPHERICAL HARMONIC TRIAL AND WEIGHT FUNCTION
* SUBSCRIPTS.
**************************************************************
PRINT*,'  TOTAL INTEGRAL VALUES IN MATRIX FORM, OF THE SPHERICAL
PRINT*,   HARMONIC TRIAL AND WEIGHT FUNCTIONS USED IN THE
PRINT*,  GALERKIN SOLUTION OF THE EVEN-PARITY BOLTZMANN EQUATION
PRINT*,   THESE VALUES ARE SELECTED PRODUCTS OF THE ASSOCIATED
PRINT*,   LEGENDRE POLYNOMIALS AND ANGULAR INTEGRALS WHICH WERE
PRINT*,   COMPUTED EARLIER. THEY REPRESENT THE SCATTERING AND
PRINT*,  NON-SCATTERING ANGULAR INTEGRAL KERNELS WHICH ARE FORMED
PRINT*,   WHEN SPHERICAL HARMONICS ARE USED AS THE ANGULAR TRIAL
PRINT*,   AND WEIGHT FUNCTIONS IN THE GALERKIN SOLUTION.'
PRINT*,
PRINT*,
DO 220 I=1,29
IW=[illegible]
IF (I.EQ.1) THEN
ISA=1
IPA=1
GO TO 10
ELSE IF (I.EQ.2) THEN
ISA=2
IPA=1
GO TO 10
ELSE IF (I.EQ.[illegible]) THEN
ISA=[illegible]
IPA=1
GO TO 10
ELSE IF (I.EQ.4) THEN
ISA=[illegible]
IPA=1
GO TO [illegible]
ELSE IF (I.EQ.5) THEN
ISA=4
IPA=1
```

```
GO TO 10
ELSE IF (I.EQ.6) THEN
ISA=5
IPA=2
GO TO 10
ELSE IF (I.EQ.7) THEN
ISA=3
IPA=2
GO TO 10
ELSE IF (I.EQ.8) THEN
ISA=5
IPA=2
GO TO 32
ELSE IF (I.EQ.9) THEN
ISA=6
IPA=4
GO TO 10
ELSE IF (I.EQ.19) THEN
ISA=6
IPA=6
GO TO 10
ENDIF
GO TO 36
DO 30 K=0,LMAX
DO 30 N=0,K
IT=0
IW=IW+1
DO 30 L=0,LMAX
DO 30 M=0,L
IT=IT+1
CA(IW,IT,I)=CL(K,N)*CL(L,M)*SA(M,N,ISA)*PL(IW,IT,IPA)
CONTINUE
GO TO 38
DO 35 K=0,LMAX
DO 35 N=0,K
IT=0
IW=IW+1
DO 35 L=0,LMAX
DO 35 M=0,L
IT=IT+1
CA(IW,IT,I)=CL(K,N)*CL(L,M)*SA(N,M,ISA)*PL(IW,IT,IPA)
CONTINUE
IF(I.LE.9.OR.I.EQ.19)GO TO 200
IF (I.EQ.21.OR.I.EQ.29) THEN
DO 40 K=0,LMAX
DO 40 N=0,K
IT=0
IW=IW+1
DO 40 L=0,LMAX
DO 40 M=0,L
IT=IT+1
IF (I.EQ.21) THEN
TEMP1=SA(M,N,1)+[illegible]
CA(IW,IT,I)=CL(K,N)*CL(L,M)*(TEMP1*PL(IW,IT,[illegible]))
GO TO 40
ELSE IF (I.EQ.29) THEN
```

```
TEMP1=PL(IW,IT,7)+PL(IW,IT,8)
CA(IW,IT,I)=CL(K,N)*CL(L,M)*TEMP1*SH(M,N,6)
ENDIF
CONTINUE
GO TO 200
ELSE IF (I.EQ.22) THEN
ISA=3
IPA=3
GO TO 45
ELSE IF (I.EQ.23) THEN
ISA=5
IPA=3
GO TO 45
ELSE IF (I.EQ.24) THEN
ISA=6
IPA=5
GO TO 45
ENDIF
GO TO 55
DO 50 K=0,LMAX
DO 50 N=0,K
IT=0
IW=IW+1
DO 50 L=0,LMAX
DO 50 M=0,L
IT=IT+1
MI=L-M
A=(1.-(-1.)**MI)
IF(M.EQ.0)A=A/2.
CA(IW,IT,I)=CL(L,M)**2*CL(K,N)*SH(M,N,ISA)*PL(IW,IT,IPA)*A*XI(L)
IF(I.GE.22.AND.I.LE.24)GO TO 200
CONTINUE
IF (I.EQ.28) THEN
DO 60 K=0,LMAX
DO 60 N=0,K
IT=0
IW=IW+1
DO 60 L=0,LMAX
DO 60 M=0,L
IT=IT+1
MI=L-M
A=(1.+(-1.)**MI)
IF(M.EQ.0)A=A/2.
CA(IW,IT,I)=CL(L,M)**2*CL(K,N)*SH(M,N,6)*PL(IW,IT,6)*A*XI(L)
GO TO 200
ENDIF
IF (I.EQ.10) THEN
IIA=[illegible]
IIB=[illegible]
IID=[illegible]
IIE=[illegible]
IPA=[illegible]
IPB=[illegible]
GO TO 1[illegible]
ELSE IF (I.EQ.11) THEN
IIA=[illegible]
```

```
ISB=5
ISD=7
ISE=9
IPA=3
IPB=3
GO TO 130
ELSE IF (I.EQ.12) THEN
ISA=3
ISB=6
ISD=7
ISE=8
IPA=5
IPB=3
GO TO 130
ELSE IF (I.EQ.13) THEN
ISA=5
ISB=3
ISD=9
ISE=7
IPA=3
IPB=3
GO TO 130
ELSE IF (I.EQ.14) THEN
ISA=5
ISB=5
ISD=9
ISE=9
IPA=3
IPB=3
GO TO 130
ELSE IF (I.EQ.15) THEN
ISA=5
ISB=6
ISD=9
ISE=8
IPA=5
IPB=[illegible]
GO TO 1[illegible]
ELSE IF (I.EQ.16) THEN
ISA=[illegible]
ISB=3
ISD=8
ISE=7
IPA=3
IPB=5
GO TO 1[illegible]
ELSE [illegible] .1[illegible] THEN
[illegible]
[illegible]
[illegible]
[illegible]
[illegible]
IPB=5
GO TO 1[illegible]
ELSE IF [illegible] THEN
ISA=[illegible]
```

```
IIB=6
IID=8
IIE=8
IPA=5
IPB=5
GO TO 130
ELSE IF (I.EQ.20) THEN
IIA=6
IIB=6
IID=8
IIE=8
IPA=6
IPB=6
GO TO 130
ENDIF
GO TO 150
DO 145 K=0,LMAX
DO 145 N=0,K
IT=0
IW=IW+1
DO 145 L=0,LMAX
DO 145 M=0,L
IR=0
IT=IT+1
CA(IW,IT,I)=0.
DO 145 JR=0,LMAX
TEMP=0.
XKU=XIOIL(JR)/(DIST-XIODL(JR))
IF(I.EQ.20)XKU=XIEVL(JR)
DO 140 JI=0,JR
IR=IR+1
IA=2
IF(JI.EQ.0)IA=IA/2
TEMP=IA*CL(K,N)*CL(L,M)*CL(JR,JI)**2*(IH(JI,N,IIA)*IH(JI,M,IIB)+IH
1(JI,N,IID)*IH(JI,M,IIE))*PL(IT,IR,IPA)*PL(IW,IR,IPB)+TEMP
CONTINUE
CA(IW,IT,I)=TEMP*XKU+CA(IW,IT,I)
CONTINUE
CONTINUE
IF(I.GE.16.AND.I.LE.20)GO TO 10
IF (I.EQ.25) THEN
IIA=3
IIB=6
IID=7
IIE=[illegible]
IPA=[illegible]
IPB=[illegible]
GO TO [illegible]
ELSE IF (I.EQ.[illegible]) THEN
IIA=[illegible]
IIB=[illegible]
IID=[illegible]
IIE=[illegible]
IPA=[illegible]
IPB=[illegible]
GO TO [illegible]
```

```
      ELSE IF (I.EQ.27) THEN
      ISA=6
      ISB=6
      ISD=8
      ISE=8
      IPA=5
      IPB=6
      ENDIF
      DO 175 K=0,LMAX
      DO 175 N=0,K
      IT=0
      IW=IW+1
      DO 175 L=0,LMAX
      DO 175 M=0,L
      IP=0
      IT=IT+1
      CA(IW,IT,I)=0.
      DO 175 JR=0,LMAX
      TEMP=0.
      XKU=XSOOL(JR)/(SIGT-XSOOL(JR))
      DO 170 JS=0,JR
      IP=IP+1
      MS=L-M
      A=2*(1.-(-1.)**MS)
      IF(JS.EQ.0.OR.M.EQ.0)A=A/2
      TEMP=CL(L,M)*CL(K,N)*CL(JR,JS)**2*(SH(JS,N,ISA)*SH(JS,M,ISB)+SH(JS
     1,N,ISD)*SH(JS,M,ISE))*PL(IT,IP,IPA)*PL(IW,IP,IPB)*A+TEMP
      CONTINUE
      CA(IW,IT,I)=CA(IW,IT,I)+TEMP*XKU*XS(L)
      CONTINUE
      PRINT*,' MATRIX VALUES FOR ANGLE INTEGRAL=',I
      DO 210 IW=1,KT
      PRINT*,(' ',CA(IW,IT,I),IT=1,KT)
      PRINT*,
      PRINT*,
      CONTINUE
      RETURN
      END
      SUBROUTINE COEFF(LMAX,CL)
      DIMENSION CL(0:3,0:3)
      ****************************************************************
      * THIS ROUTINE COMPUTES THE SPHERICAL HARMONIC EXPANSION         *
      * COEFFICIENTS OF  NORMALIZATION CONSTANTS.
      ****************************************************************
      REAL INF,IDF
      [illegible]
      [illegible]
      [illegible] GO TO [illegible]
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      IF(INT.EQ.0) GO TO [illegible]
      [illegible]
      [illegible]
      [illegible]
```

```
IDF=IDF*I
FT=INF/IDF
GO TO 100
FT=1.
CL(L,M)=SQRT((2*L+1)/(4*(4*ATAN(1.))))*FT)
CONTINUE
RETURN
END
SUBROUTINE SPLINE(SPX,NXS,TOL,KOUNT)
DIMENSION PNX(-2:7),SPX(7,7,6)
COMMON/A1/PNX,I/A3/JR,JT/B4/L,K
*****************************************************************
* THIS ROUTINE COMPUTES THE BICUBIC SPLINE INTEGRALS BY CALLING **
* A TEN POINT NEWTON-COTES INTEGRATION ROUTINE.
*****************************************************************
DO 90 JR=1,NXS
DO 90 JC=1,NXS
SPX(JR,JC,I)=0.0
JT=JC-JR
IF(ABS(JT).GT.3)GO TO 90
KF=4
IF (JT.EQ.0) THEN
KI=1
GO TO 5
ELSE IF (JT.EQ.1) THEN
KI=2
GO TO 5
ELSE IF (JT.EQ.2) THEN
KI=3
GO TO 5
ELSE IF (JT.EQ.3) THEN
KI=4
GO TO 5
ENDIF
KI=1
IF (JT.EQ.-1) THEN
KF=3
GO TO 5
ELSE IF (JT.EQ.-2) THEN
KF=2
GO TO 5
ELSE IF (JT.EQ.-3) THEN
KF=1
GO TO 5
ENDIF
DO 10 K=KI,KF
[illegible]
[illegible]
IF(L.LT.0)GO TO 10
IF(L.GT.1)GO TO 10
CALL QUAD(AMP(L),AMP(L+1),TOL,TV,KOUNT)
[illegible]
CONTINUE
CONTINUE
[illegible]
[illegible]
```

```
DO 100 MR=1,NXC
PRINT*,'         ',(SPX(MR,MC,I),MC=1,NXC)
PRINT*,' '
PRINT*,' '
RETURN
END
FUNCTION SPF(IP,JP,X1,X2,X3,X4,X)
**********************************************************************
* THIS ROUTINE SELECTS AND COMPUTES THE BICUBIC SPLINE FUNCTIONS *
* THAT ARE BEING INTEGRATED.
**********************************************************************
A=(X4-X)
Z=A**3
Z1=-3*A**2.
IF (JP.EQ.4) THEN
IF (IP.EQ.1) THEN
SPF=Z
RETURN
ELSE IF (IP.EQ.2) THEN
SPF=Z1
RETURN
ELSE IF (IP.EQ.3) THEN
SPF=Z+X*Z1
RETURN
ENDIF
ENDIF
B=X3-X
Y=Z-4*B**3
Y1=12.*B**2+Z1
IF (JP.EQ.3) THEN
IF (IP.EQ.1) THEN
SPF=Y
RETURN
ELSE IF (IP.EQ.2) THEN
SPF=Y1
RETURN
ELSE IF (IP.EQ.3) THEN
SPF=Y+X*Y1
RETURN
ENDIF
ENDIF
C=X2-X
V=Y+6*C**3
V1=Y1-18.*C**2
IF (JP.EQ.2) THEN
IF (IP.EQ.1) THEN
SPF=V
RETURN
ELSE IF (IP.EQ.2) THEN
SPF=V1
RETURN
ELSE IF (IP.EQ.3) THEN
SPF=V+X*V1
RETURN
ENDIF
ENDIF
```

```
D=X1-X
W=V-4*D**3
W1=V1+12.*D**2
IF (JP.EQ.1) THEN
IF (IP.EQ.1) THEN
SPF=W
RETURN
ELSE IF (IP.EQ.2) THEN
SPF=W1
RETURN
ELSE IF (IP.EQ.3) THEN
SPF=W+X*W1
ENDIF
ENDIF
RETURN
END
SUBROUTINE SOURCE(SVX,NXS,TOL,KOUNT)
DIMENSION SVX(7,5,3),PNX(-2:7)
COMMON/A1/PNX,I /A4/KS,IH,LP/B4/L,K
*****************************************************************
* THIS ROUTINE SELECTS AND COMPUTES THE INTERPOLATED SOURCE       *
* INTEGRAL BY CALLING A TEN POINT NEWTON COTES INTEGRATION ROUTINE
*****************************************************************
DO 80 LP=1,NXS
DO 80 LC=1,NXS-2
SVX(LP,LC,I)=0.0
LY=LC-LP
IF(LY.GT.1.OR.LY.LT.-3)GO TO 80
KF=4
IF (LY.EQ.1) THEN
KI=4
GO TO 10
ELSE IF(LY.EQ.0) THEN
KI=3
GO TO 10
ENDIF
IF (LY.EQ.-1) THEN
KI=[illegible]
KF=[illegible]
GO TO 10
ELSE IF (LY.EQ.-2) THEN
KI=1
KF=2
GO TO 10
ELSE IF (LY.EQ.-3) THEN
KI=1
KF=1
ENDIF
IH=1
IF(LY.EQ.-[illegible])IH=[illegible]
DO [illegible] K=KI,KF
[illegible]
LB=LP-N[illegible]+K[illegible]
IF [illegible]
IF(KS.GT.1)GO TO [illegible]
CALL [illegible]
```

```
SVX(LR,LC,I)=SVX(LR,LC,I)+TV
IH=IH+1
CONTINUE
PRINT*,' MATRIX SOURCE INTEGRAL=',I
DO 90 MR=1,NXS
PRINT*,(' ',SVX(MR,MC,I),MC=1,NXS-2)
PRINT*,' '
RETURN
END
FUNCTION HIF(IH,X1,X2,X)
*****************************************************************
* THIS ROUTINE COMPUTES THE LINEAR LAGRANGE POLYNOMIALS WHICH ***
* ARE BEING INTEGRATED AS A PART OF THE SOURCE INTEGRALS.
*****************************************************************
IF (IH.EQ.2) THEN
HIF=(X2-X)/(X2-X1)
RETURN
ELSE IF (IH.EQ.1) THEN
HIF=(X-X1)/(X2-X1)
ENDIF
RETURN
END
SUBROUTINE DIRECT(LMAX,APD,PNZ,PNR,NRS,NZS,SIGT,HB,YD,AIH)
DIMENSION APD(5,5,3),PNZ(-2:7),PNR(-2:7)
*****************************************************************
* THIS ROUTINE COMPUTES THE DIRECT SOURCE POINT VALUES WHICH ARE *
* USED IN THE FIRST COLLISION SOURCE INTERPOLATION.
*****************************************************************
PRINT*,' '
PRINT*,'  INTERPOLATION POINT VALUES.ELEMENT (I,J) IS FOR POINT (Z
1,R)'
PRINT*,' '
IW=0
DO 50 L=0,LMAX
DO 50 M=0,L
IW=IW+1
DO 40 IT=1,NZS-2
DO 40 I=1,NRS-2
ZH=PNZ(IT-1)-HB
RZH=SQRT(PNR(I-1)**2+ZH**2)
IF(RZH.EQ.0)GO TO 60
UD=ZH/RZH
IF(UD.EQ.0)GO TO 20
TAU=SIGT*(EXP(-HB/AIH)-EXP(-PNZ(IT-1)/AIH))*AIH/UD
GO TO 30
TAU=SIGT*EXP(-PNZ(IT-1)/AIH)*PNR(I-1)
APD(IT,I,IW)=YD*EXP(-TAU)/(16.*ATAN(1.)*RZH**2)*ALF(UD,L,M)*EXP(-
1PNZ(IT-1)/AIH)
CONTINUE
PRINT*,'  MATRIX VALUES FOR INTERPOLATION POINT VALUES FOR LEGENDR
1E POLYNOMIALS= ',IW
PRINT*,
DO 45 MR=1,NZS-2
PRINT*,(' ',APD(MR,J,IW),J=1,NRS-2)
PRINT*,
CONTINUE
```

```
      GO TO 70
      PRINT*,' IMPROPER INPUT DATA.A NODE CANNOT BE AT THE BURST POINT,Z
     1= ',PNZ(IT-1)
      STOP
      RETURN
      END
      SUBROUTINE BVEC(APD,SVZ,SVR,SB,NZS,NRS,LMAX,CA,SIGT,KT,NT)
      DIMENSION APD(5,5,3),SVZ(7,5,3),SVR(7,5,3),SB(50),CA(3,3,30)
*****************************************************************
* THIS ROUTINE ASSEMBLES THE PROBLEM SOURCE VECTOR.
*****************************************************************
      PRINT*,' '
      PRINT*,' SOURCE MATRIX COLUMN VECTOR.'
      PRINT*,' '
      IS=0
      DO 90 JZ=1,NZS
      DO 90 JR=1,NRS
      JA=0
      DO 80 JL=0,LMAX
      DO 80 JM=0,JL
      JA=JA+1
      IS=IS+1
      SB(IS)=0.
      DO 75 N=1,7
      SC=1.0
      TEMP3=0.
      IA=0
      DO 70 IL=0,LMAX
      DO 70 IM=0,IL
      IA=IA+1
      TEMP2=0.
      DO 60 IZ=1,NZS-2
      DO 60 IR=1,NRS-2
      ICZ=IZ-JZ
      ICR=IR-JR
      IF(ICZ.GT.1.OR.ICZ.LT.-3)GO TO 60
      IF(ICR.GT.1.OR.ICR.LT.-3)GO TO 60
      IF (N.EQ.1) THEN
      NC=1
      NR=1
      NA=SC
      GO TO 50
      ELSE IF (N.EQ.2) THEN
      NC=1
      NR=2
      [illegible]
      [illegible]
      ELSE IF (N.EQ.3) THEN
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      ELSE IF (N.EQ.4) THEN
      [illegible]
      [illegible]
      [illegible]
```

```
GO TO 50
ELSE IF (N.EQ.5) THEN
NZ=1
NR=2
NA=26
GO TO 50
ELSE IF (N.EQ.6) THEN
NZ=2
NR=3
NA=27
GO TO 50
ELSE IF (N.EQ.7) THEN
NZ=3
NR=3
NA=28
ENDIF
TEMP1=SVZ(JZ,IZ,NZ)*SVR(JR,IR,NR)*APD(IZ,IR,IA)*CA(JA,IA,NA)
TEMP2=TEMP1+TEMP2
CONTINUE
TEMP3=TEMP2+TEMP3
IF(NA.EQ.23.OR.NA.EQ.26)SC=-1.0
IF(N.EQ.7)GO TO 72
TEMP3=TEMP3*8*ATAN(1.)/SIGT*SC
GO TO 75
TEMP3=TEMP3*8*ATAN(1.)*SC
SB(IS)=TEMP3+SB(IS)
CONTINUE
PRINT*,'   ',KT,'  ELEMENT(S) TO ELEMENT NUMBER=',IS
PRINT*,'/  ',(SB(KS),KS=IS-(KT-1),IS)
CONTINUE
PRINT*,'  '
PRINT*,'  '
PRINT*,'  '
RETURN
END
SUBROUTINE STIFF(CA,SPR,SPZ,NZS,NRS,SIGT,AS,PNR,PNZ,LMAX,NT)
DIMENSION CA(3,3,30),SPR(7,7,6),SPZ(7,7,5),AS(50,50),PNR(-2:7),P
1NZ(-3:7)
************************************************************
THIS ROUTINE ASSEMBLES THE PROBLEM COEFFICIENT OR STIFFNESS MATRIX
************************************************************
DO 20 J=1,NT
DO 20 K=1,NT
AS(J,K)=0.0
KJ=0
DO 50 JZ=1,NZS
DO 40 JR=1,NRS
JA=0
DO 40 JL=0,LMAX
DO 40 M=0,JL
[illegible]
[illegible]
IJ=0
DO 50 IZ=1,NZS
DO 50 IR=1,NRS
IA=0
```

```
DO 50 IL=0,LMAX
DO 50 IM=0,IL
IA=IA+1
IJ=IJ+1
TEMP1=0.
TEMP2=0.
LD=JS-IS
MF=JR-IR
IF(ABS(LD).GT.3)GO TO 33
IF(ABS(MF).GT.3)GO TO 33
DO 32 N=1,19
NE=2
IF (N.EQ.1) THEN
NR=1
NS=1
GO TO 30
ELSE IF (N.EQ.2) THEN
NR=2
NS=1
NE=1
GO TO 30
ELSE IF (N.EQ.3) THEN
NR=4
NS=2
GO TO 30
ELSE IF (N.EQ.4) THEN
NR=2
NS=1
NE=1
GO TO 25
ELSE IF(N.EQ.5) THEN
NR=3
NS=1
GO TO 30
ELSE IF (N.EQ.6) THEN
NR=5
NS=2
NE=1
GO TO [illegible]
ELSE IF (N.EQ.7) THEN
NR=4
NS=2
GO TO 31
ELSE IF (N.EQ.8) THEN
NR=5
NS=[illegible]
NE=1
[illegible]
ELSE IF (N.EQ.[illegible]) THEN
[illegible]
[illegible]
[illegible]
ELSE IF (N.EQ.10) THEN
NR=1
[illegible]
[illegible]
```

```
ELSE IF (N.EQ.11) THEN
NR=2
NZ=1
NE=1
GO TO 30
ELSE IF (N.EQ.12) THEN
NR=4
NZ=2
GO TO 30
ELSE IF (N.EQ.13) THEN
NR=2
NZ=1
NE=1
GO TO 25
ELSE IF (N.EQ.14) THEN
NR=3
NZ=1
GO TO 30
ELSE IF (N.EQ.15) THEN
NR=5
NZ=2
NE=1
GO TO 30
ELSE IF (N.EQ.16) THEN
NR=4
NZ=2
GO TO 21
ELSE IF (N.EQ.17) THEN
NR=5
NZ=2
NE=1
GO TO 23
ELSE IF (N.EQ.18) THEN
NR=6
NZ=3
GO TO 30
ENDIF
TEM=IFR(IR,JR,NR)*IFZ(IZ,JZ,NZ)
GO TO [illegible]2
TEM=IFR(JR,IR,NR)*IFZ(IZ,JZ,NZ)
GO TO 32
TEM=IFR(IR,JR,NR)*IFZ(JZ,IZ,NZ)
GO TO 32
TEM=IFR(JR,IR,NR)*IFZ(JZ,IZ,NZ)
TEMP1=TEM*CA(JA,IA,N)*(-1)**NE+TEMP1
TEMP1=TEMP1*8*ATAN(1.)/DIST
TEMP2=IFR(JR,IR,6)*IFZ(JZ,IZ,4)*(A(JA,IA,19)*8*ATAN(1.))*DIST
TEMP2=IFR(JR,IR,6)*IFZ(JZ,IZ,4)*CA(JA,IA,20)*8*ATAN(1.)-TEMP2
CONTINUE
IF (IZ.GT.3.OR.IZ.GT.3) GO TO [illegible]
IF (ABS(NE).GT.[illegible]) GO TO [illegible]
IF ([illegible].EQ.1) THEN
L1=4
IF (L2.[illegible]) THEN
L2=4
GO TO [illegible]
```

```
ELSE IF (LD.EQ.-1) THEN
L2=3
GO TO 35
ELSE  IF (LD.EQ.-2) THEN
L2=2
GO TO 35
ENDIF
ELSE IF (J2.EQ.2) THEN
L1=3
IF (LD.EQ.0) THEN
L2=3
GO TO 35
ELSE IF (LD.EQ.1) THEN
L2=4
GO TO 35
ELSE IF (LD.EQ.-1) THEN
L2=2
GO TO 35
ENDIF
ELSE IF (J2.EQ.3) THEN
L1=2
IF (LD.EQ.0) THEN
L2=2
GO TO 35
ELSE IF (LD.EQ.1) THEN
L2=3
GO TO 35
ELSE IF (LD.EQ.2) THEN
L2=4
ENDIF
ENDIF
PBZI=IPF(1,L1,PNZ(JZ-3),PNZ(JZ-2),PNZ(JZ-1),PNZ(JZ),PNZ(0))*IPF(1,
1L2,PNZ(IZ-3),PNZ(IZ-2),PNZ(IZ-1),PNZ(IZ),PNZ(0))
GO TO 40
PBZI=0.
ND=NZI-JZ
MD=NZI-IZ
IF(ND.GT.3.OR.MD.GT.3)GO TO 48
IF(ABS(MD).GT.3)GO TO 4[illegible]
CALL [illegible](D,JZ,IZ,PNZ,PBZI,NZI)
GO TO 4[illegible]
PBZI=0.
ND=NRI-JR
MD=NRI-IR
IF(ND.GT.2.OR.MD.GT.2)GO TO 47
IF(ABS(LD).GT.2)GO TO 47
CALL [illegible](JR,IR,PNR,PBRI,NRI)
GO TO [illegible]
[illegible]
TEMP[illegible]
TEMP1=[illegible]
TEMP3=[illegible]
[illegible]=TEMP1-TEMP2+TEMP3
CONTINUE
RETURN
END
```

```
SUBROUTINE BOUND(JX,IX,FN(),TEMP,NXX)
DIMENSION FN(-2:7)
***********************************************************************
* THIS ROUTINE SELECTS AND COMPUTES THE VALUES OF THE BICUBIC         *
* SPLINE FUNCTIONS AT THE OUTER RADIUS AND TOP SURFACE OF THE         *
* PROBLEM CYLINDER.THESE VALUES ARE REQUIRED IN THE EVALUATION OF
* THE SURFACE INTEGRAL TERMS.
***********************************************************************
LI=NXX-JX
LD=JX-IX
IF (LI.EQ.0) THEN
L1=1
IF (LD.EQ.0) THEN
L2=1
GO TO 40
ELSE IF (LD.EQ.1) THEN
L2=2
GO TO 40
ELSE IF (LD.EQ.2) THEN
L2=3
GO TO 40
ENDIF
ELSE IF (LI.EQ.1) THEN
L1=2
IF (LD.EQ.0) THEN
L2=2
GO TO 40
ELSE IF(LD.EQ.-1) THEN
L2=1
GO TO 40
ELSE IF (LD.EQ.1) THEN
L2=3
GO TO 40
ENDIF
ELSE IF (LI.EQ.2) THEN
L1=3
IF (LD.EQ.0) THEN
L2=[illegible]
GO TO 40
ELSE IF (LI.EQ.-[illegible]) THEN
L2=2
GO TO 40
ELSE IF (LD.EQ.-2) THEN
L2=1
ENDIF
ENDIF
TEMP=[illegible]
[illegible]
RETURN
END
[illegible]
[illegible]
***********************************************************************
* [illegible] MATRI[illegible]
* AND [illegible] CONDUCTANCE.
***********************************************************************
```

```
PRINT*,'  MATRIX CHECK FOR DIAGONAL DOMINANCE.'
PRINT*,'  '
PRINT*,'  ROW     DIAGONAL ELEMENT      SUM OF ROW ELEMENTS.'
PRINT*,' '
DO 40 I=1,NT
TEMP=0.0
DO 30 J=1,NT
TEMP=TEMP+ABS(AS(I,J))
TEMP=TEMP-ABS(AS(I,I))
PRINT*,'    ',I,'     ',AS(I,I),'         ',TEMP
PRINT*,' '
CONTINUE
PRINT*,' '
PRINT*,'  MATRIX CHECK FOR SYMMETRY.'
PRINT*,' '
DO 60 I=1,NT
DO 60 J=1,I
PRINT*,' AS(',I,',',J,')= ',AS(I,J),'           AS(',J,',',I,')=  ',A
1S(J,I)
CONTINUE
RETURN
END
SUBROUTINE SOLVE(W,SB,AS,NT,XB)
DIMENSION AS(50,50),SB(50),XA(50),XB(50)
*****************************************************************
* THIS ROUTINE SOLVES THE PROBLEM MATRICES BY THE ITERATIVE MET(HO
* OF SUCCESSIVE OVER-RELAXATION.
*****************************************************************
PRINT*,' '
PRINT*,' '
DO 20 I=1,NT
XA(I)=0.
XB(I)=0.
IT=0
IT=IT+1
DO 50 K=1,NT
TEMP=SB(K)
DO 40 J=1,NT
TEMP=TEMP-AS(K,J)*XB(J)
XB(K)=TEMP*W/AS(K,K)+XB(K)
DO 60 I=1,NT
IF(XB(I).EQ.0.)GO TO 60
TOL=(XB(I)-XA(I))/XB(I)
IF(ABS(TOL).GT..001)GO TO 70
CONTINUE
GO TO 90
CONTINUE
IF(IT.[illegible].1000)GO TO 10
DO 80 I=1,NT
[illegible]
[illegible]
PRINT*,'  THE SOLUTION HAS CONVERGED.THE FINAL TOL WAS ',TOL
PRINT*,'   THE NUMBER OF ITERATIONS WERE ',IT
PRINT*,'   SOLUTION VECTOR,[illegible] COEFFICIENT [illegible]'
PRINT*,' [illegible]
[illegible]
```

```
PRINT*,' THE PROBLEM HAS NOT CONVERGED IN ',IT,' ITERATIONS.'
PRINT*,' '
PRINT*,' THE ERROR =',TOL
PRINT*,' '
PRINT*,(' ',XB(I),I=1,NT)
RETURN
END
SUBROUTINE TFLUX(PNR,PNZ,XB,R,Z,KT,NZS,NRS,TPHI,DPHI,HB,SIGT,ASH,
1D)
DIMENSION PNZ(-2:7),PNR(-2:7),XB(50),ISPF(4,4)
***************************************************************
* THIS ROUTINE COMPUTES THE SCATTERED AND TOTAL REACTION RATE
* FLUENCE.
***************************************************************
CALL IEMAT(ISPF,PNR,PNZ,R,Z,NRS,NZS)
KZ=5
TEMP1=0.
DO 40 I=1,4
MZ=ISPF(I,1)
IF(MZ.GT.NZS)GO TO 40
KZ=KZ-1
KR=5
DO 30 J=1,4
MR=ISPF(J,2)
IF(MR.GT.NRS)GO TO 30
NF=1+KT*((MR-1)+NRS*(MZ-1))
KR=KR-1
TEMP=XB(NF)*SPF(1,KZ,PNZ(MZ-3),PNZ(MZ-2),PNZ(MZ-1),PNZ(MZ),Z)*SPF(
11,KR,PNR(MR-3),PNR(MR-2),PNR(MR-1),PNR(MR),R)
TEMP1=TEMP1+TEMP
CONTINUE
CONTINUE
A=SQRT(16.*ATAN(1.))
TPHI=A*TEMP1
ZH=Z-HB
RZH=SQRT(R**2+ZH**2)
IF(RZH.EQ.0)GO TO 80
SI=ZH/RZH
IF(SI.EQ.0.)GO TO 60
TAU=SIGT*(EXP(-HB/ASH)-EXP(-Z/ASH))*ASH/SD
GO TO 70
TAU=SIGT*EXP(-Z/ASH)*R
DPHI=YD*EXP(-TAU)/(16*ATAN(1.)*RZH**2)
GO TO 90
PRINT*,' ERROR.THE FLUX CANNOT BE COMPUTED AT THE BURST POINT.'
STOP
RETURN
END
SUBROUTINE IEMAT(ISPF,PNR,PNZ,R,Z,NRS,NZS)
DIMENSION ISPF(4,4),PNR(-2:7),PNZ(-2:7)
***************************************************************
* THIS ROUTINE COMPUTES THE VALUES OF THE FOURIER SPLINES AT THE *
* SELECTED TRACE POINTS.
***************************************************************
[illegible]
[illegible]
```

```
      DO 40 I=0,NZS-3
      IF(Z.GE.PNZ(I).AND.Z.LT.PNZ(I+1))GO TO 50
      CONTINUE
      DO 60 J=1,4
      ISPF(J,1)=I+J
      DO 70 I=0,NRS-3
      IF(R.GE.PNR(I).AND.R.LT.PNR(I+1))GO TO 80
      CONTINUE
      DO 85 J=1,4
      ISPF(J,2)=I+J
      GO TO 100
      PRINT*,'  THE SPACIAL POSITION OF',Z,' OR ',R,' IS NOT WITHIN THE
     1PROBLEM DIMENSIONS.'
      STOP
      RETURN
      END
```

Appendix K

Numerical Results

The computer subroutines which are listed in Appendix J were used to produce numerical results for varying problem spatial mesh sizes and degrees of the spherical harmonic trial function expansion. Some of these results are presented in Figures 10 through 44. They are valid for the problem parameters which were presented in Chapter V. However, the cross-sections which were used do not accurately represent the values for air at sea level. Also, the air-ground interface was not included in the problem domain and therefore all ground effects were ignored.

Because of the time constraints on this research project neither an evaluation of the accuracy of these results nor a comparison to a discrete ordinate or Monte Carlo calculation was accomplished. Therefore, the results are presented solely in an attempt to show that finite element space-angle synthesis is a viable solution technique for solving the two-dimensional steady state anisotropic Boltzmann equation. They are not meant to represent a precise and exact solution to the air-over-ground problem, but rather to demonstrate that FESAS may be a feasible alternate solution technique to Monte Carlo and discrete ordinates.

PARTICLE(NEUTRON) FLUENCES.

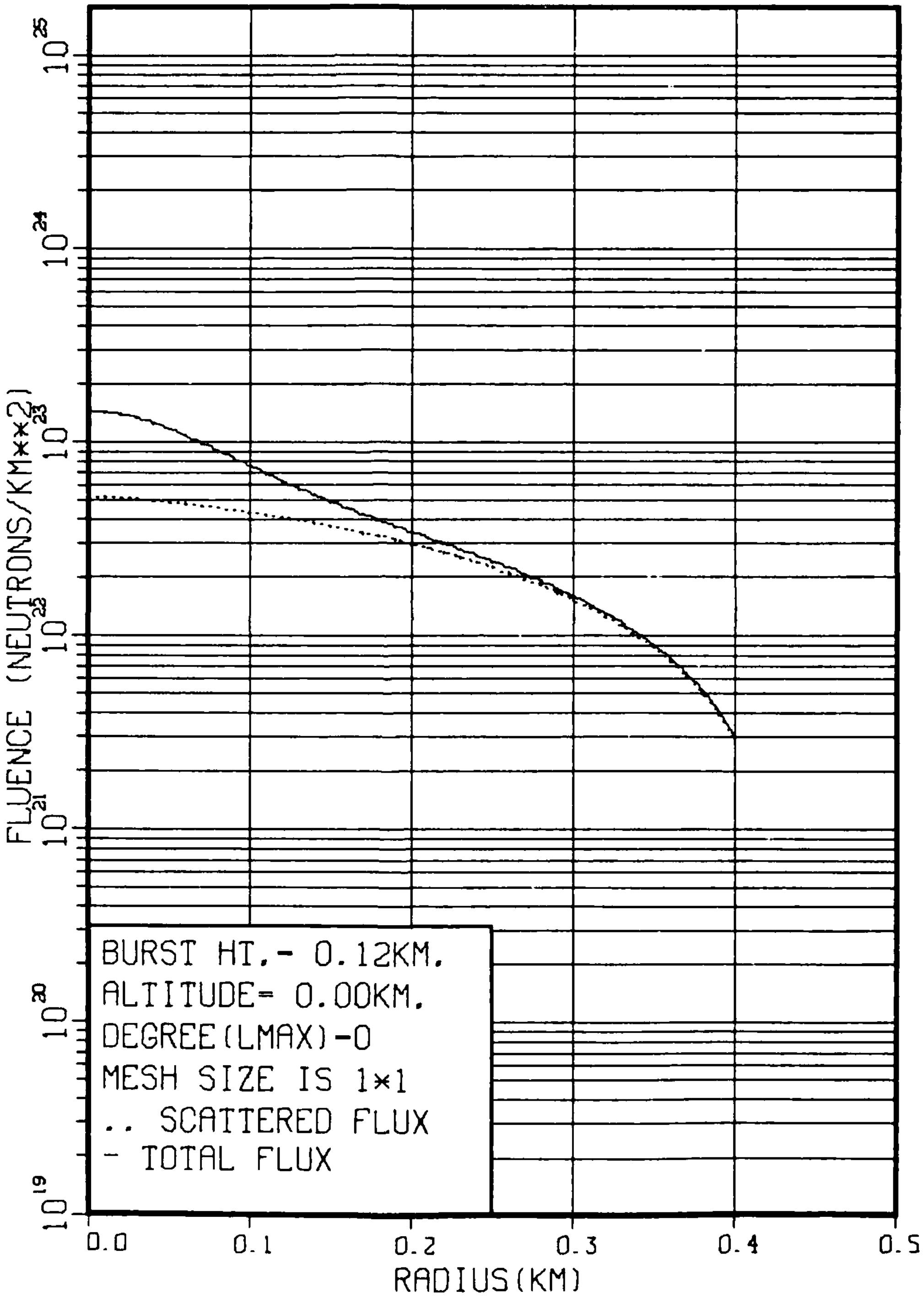


Figure 10

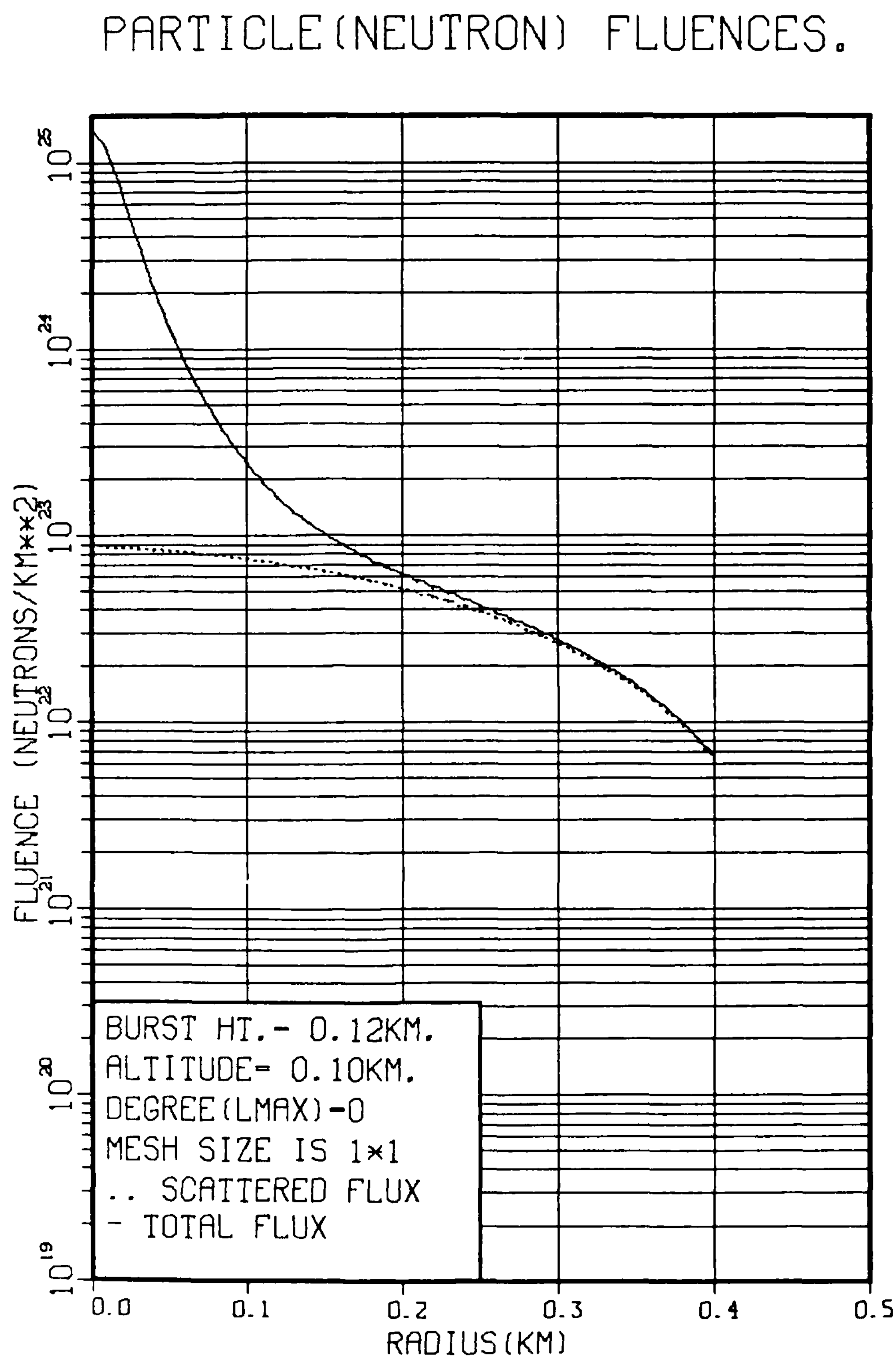

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^{25}
10^{24}
10^{23}
10^{22}
10^{21}
10^{20}
10^{19}
BURST HT.- 0.12KM.
ALTITUDE= 0.10KM.
DEGREE(LMAX)-0
MESH SIZE IS 1*1
.. SCATTERED FLUX
- TOTAL FLUX
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)

Figure 11

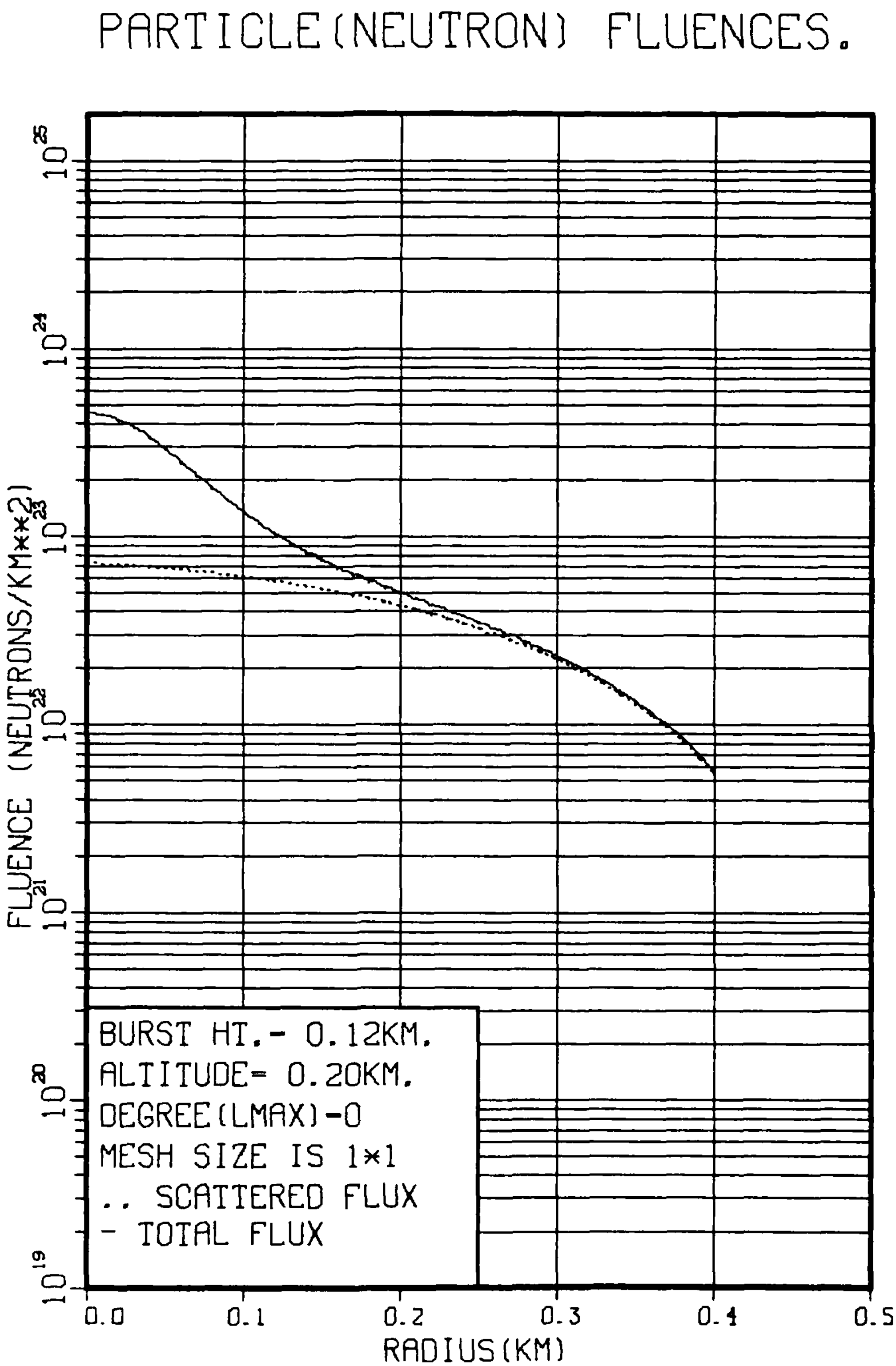

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE= 0.20KM.
DEGREE(LMAX)-0
MESH SIZE IS 1*1
.. SCATTERED FLUX
- TOTAL FLUX

Figure 12

PARTICLE(NEUTRON) FLUENCES.

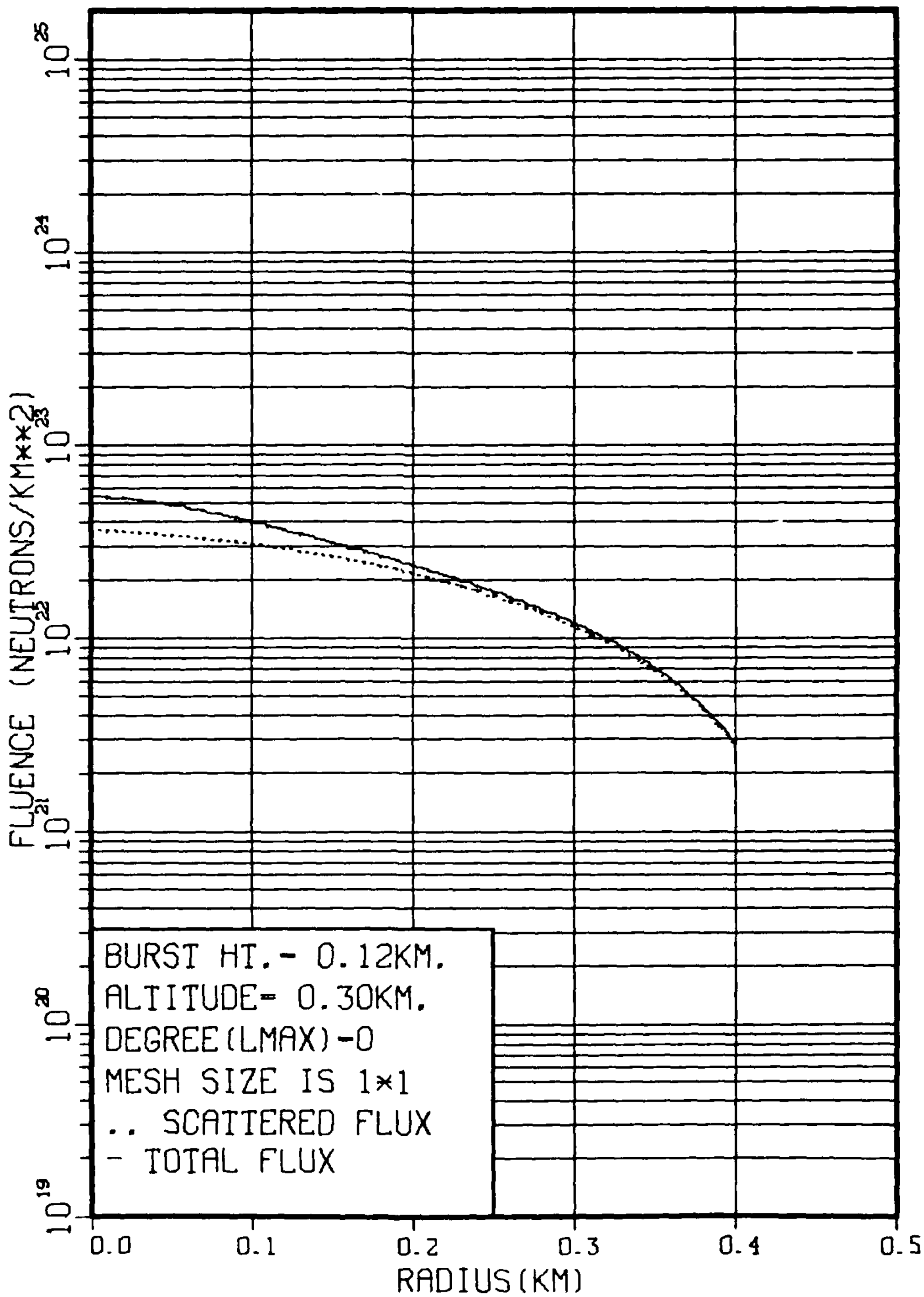


Figure 13

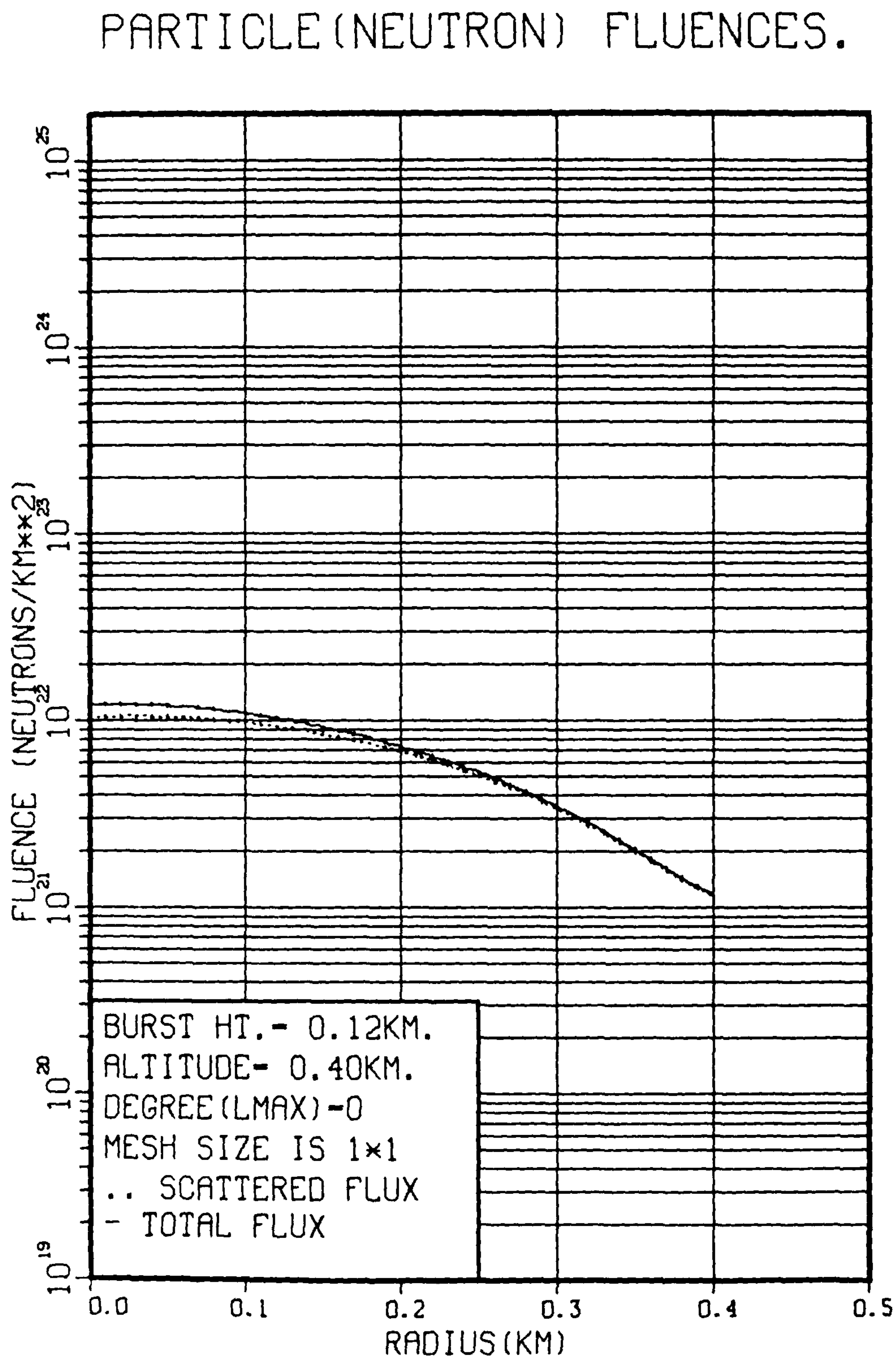
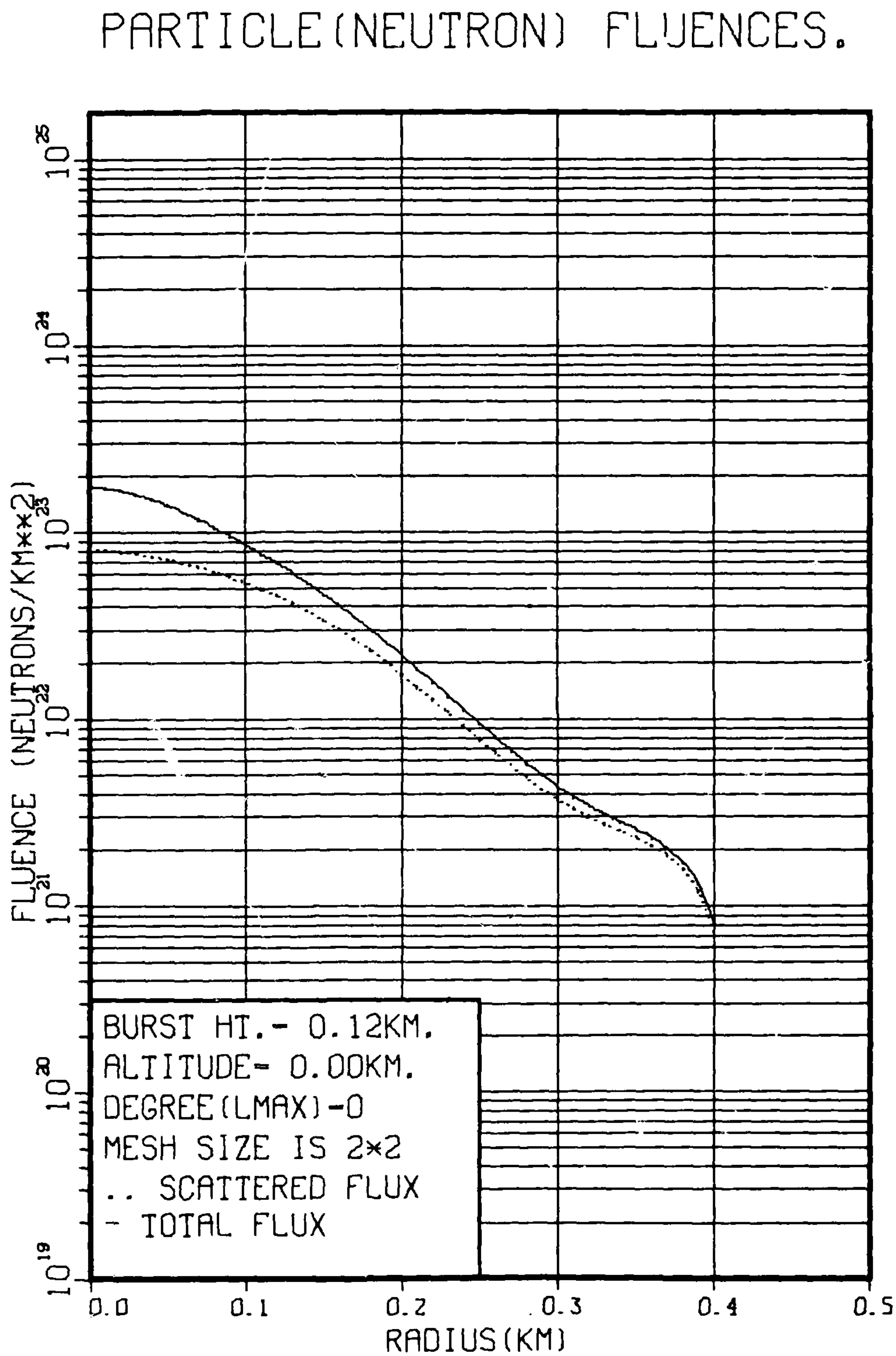

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^{25}
10^{24}
10^{23}
10^{22}
10^{21}
10^{20}
10^{19}
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE- 0.40KM.
DEGREE(LMAX)-0
MESH SIZE IS 1*1
.. SCATTERED FLUX
- TOTAL FLUX

Figure 14



PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^{25}
10^{24}
10^{23}
10^{22}
10^{21}
10^{20}
10^{19}
BURST HT.- 0.12KM.
ALTITUDE- 0.00KM.
DEGREE(LMAX)-0
MESH SIZE IS 2*2
.. SCATTERED FLUX
- TOTAL FLUX
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)

Figure 15

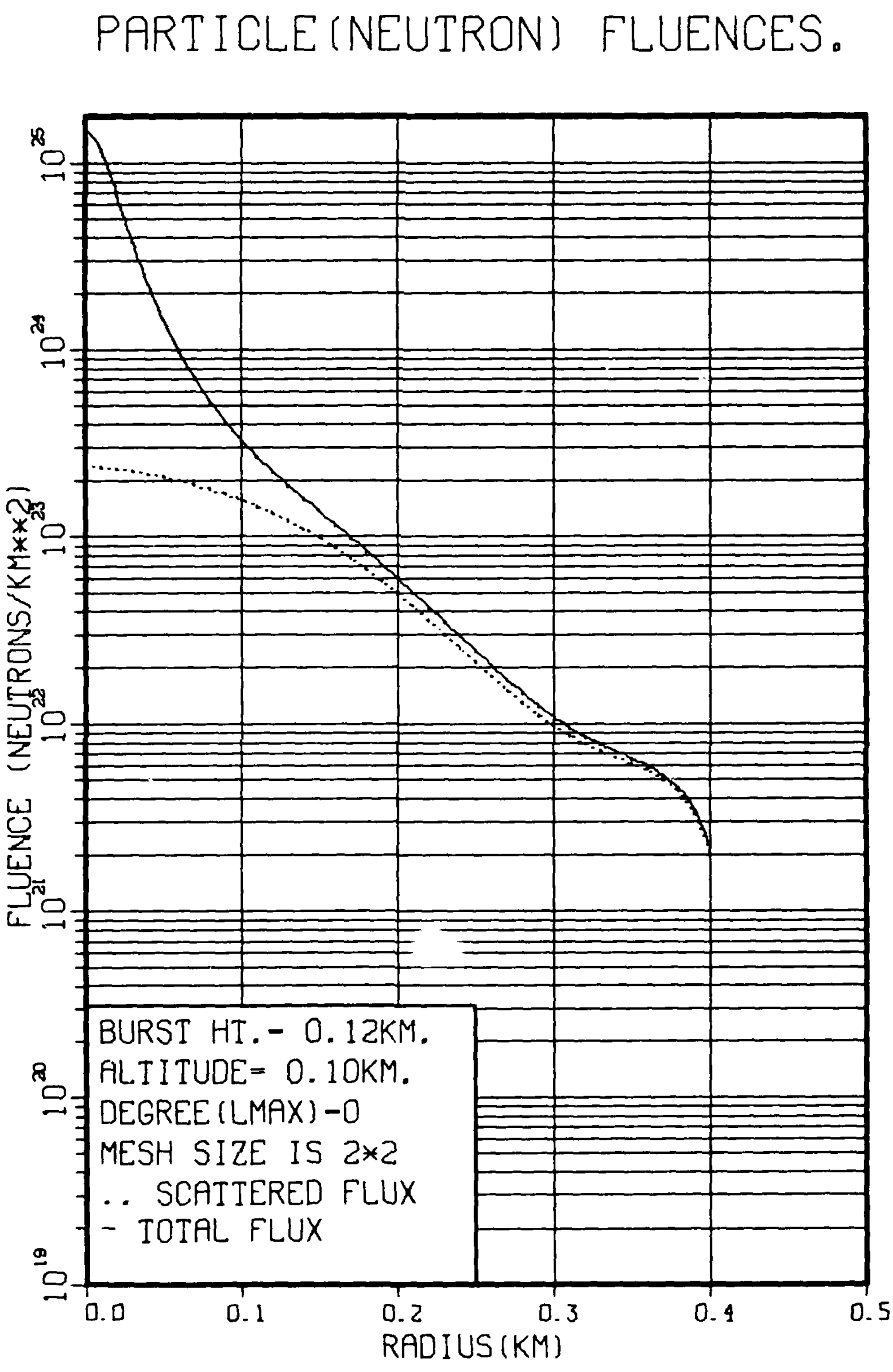

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^25
10^24
10^23
10^22
10^21
10^20
10^19
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE= 0.10KM.
DEGREE(LMAX)-0
MESH SIZE IS 2*2
.. SCATTERED FLUX
- TOTAL FLUX

Figure 16

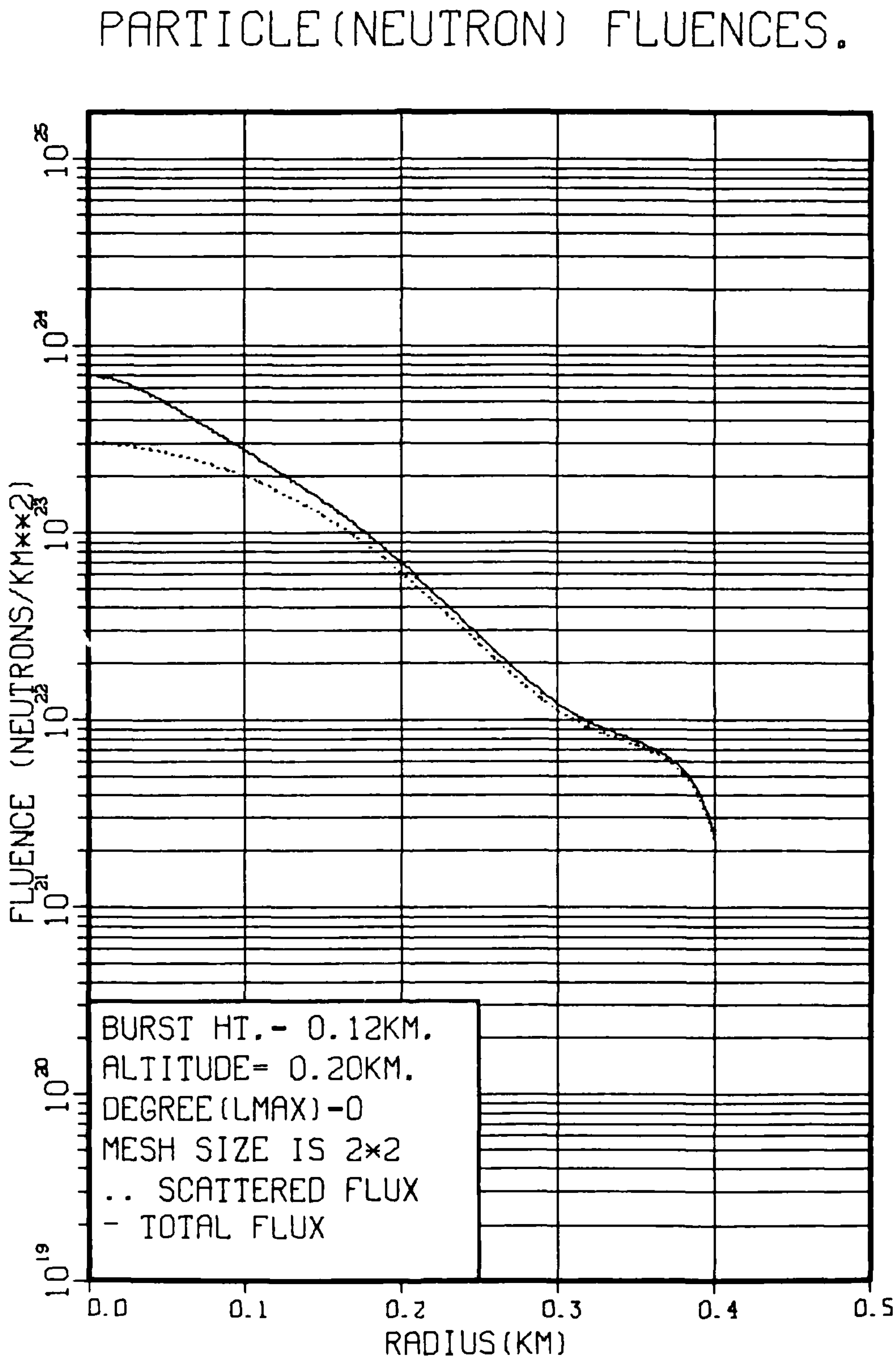

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^25
10^24
10^23
10^22
10^21
10^20
10^19
BURST HT.- 0.12KM.
ALTITUDE= 0.20KM.
DEGREE(LMAX)-0
MESH SIZE IS 2*2
.. SCATTERED FLUX
- TOTAL FLUX
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)

Figure 17

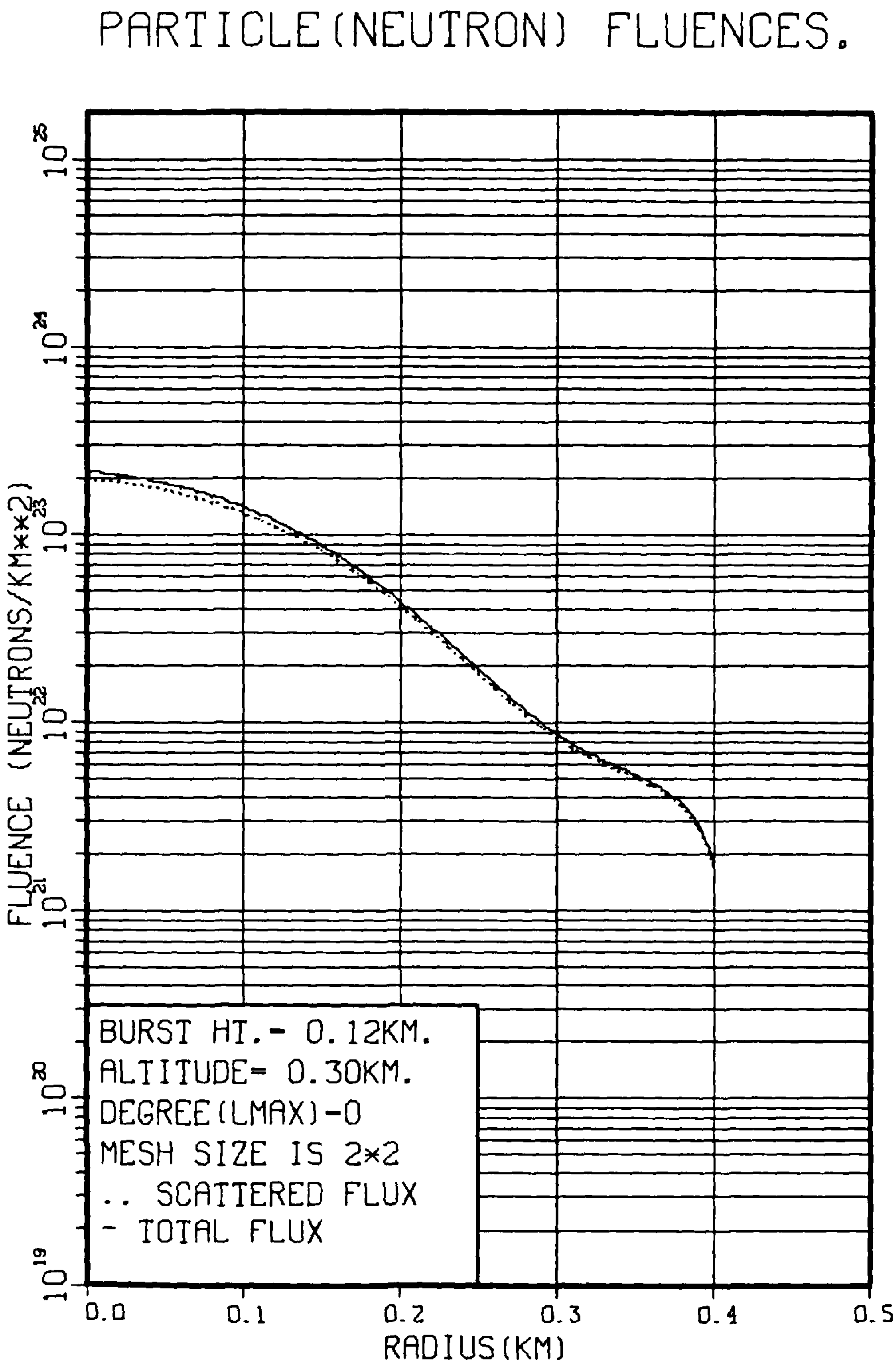

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^{25}
10^{24}
10^{23}
10^{22}
10^{21}
10^{20}
10^{19}
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE= 0.30KM.
DEGREE(LMAX)-0
MESH SIZE IS 2*2
.. SCATTERED FLUX
- TOTAL FLUX

Figure 18

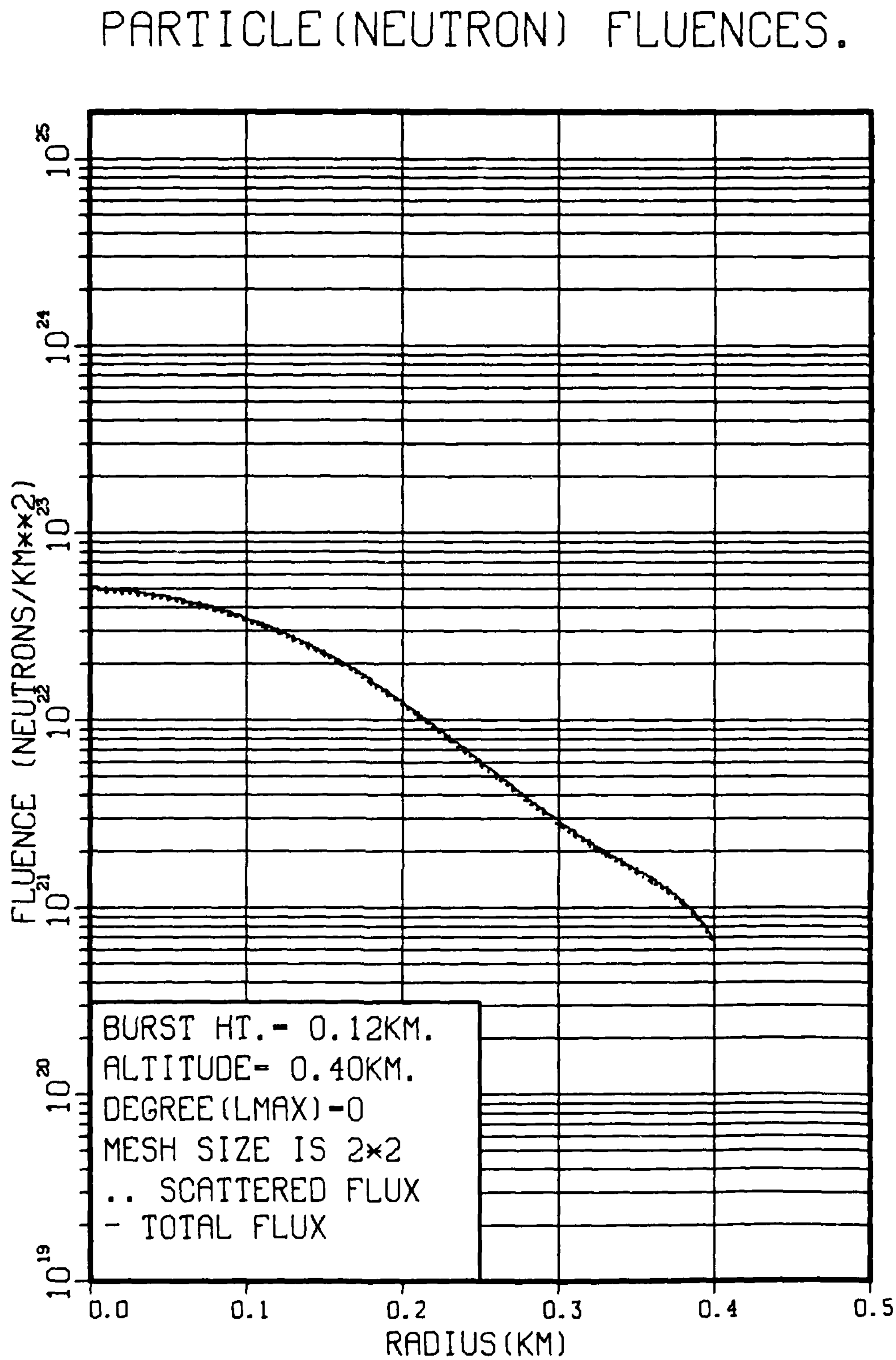

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^25
10^24
10^23
10^22
10^21
10^20
10^19
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE- 0.40KM.
DEGREE(LMAX)-0
MESH SIZE IS 2*2
.. SCATTERED FLUX
- TOTAL FLUX

Figure 19

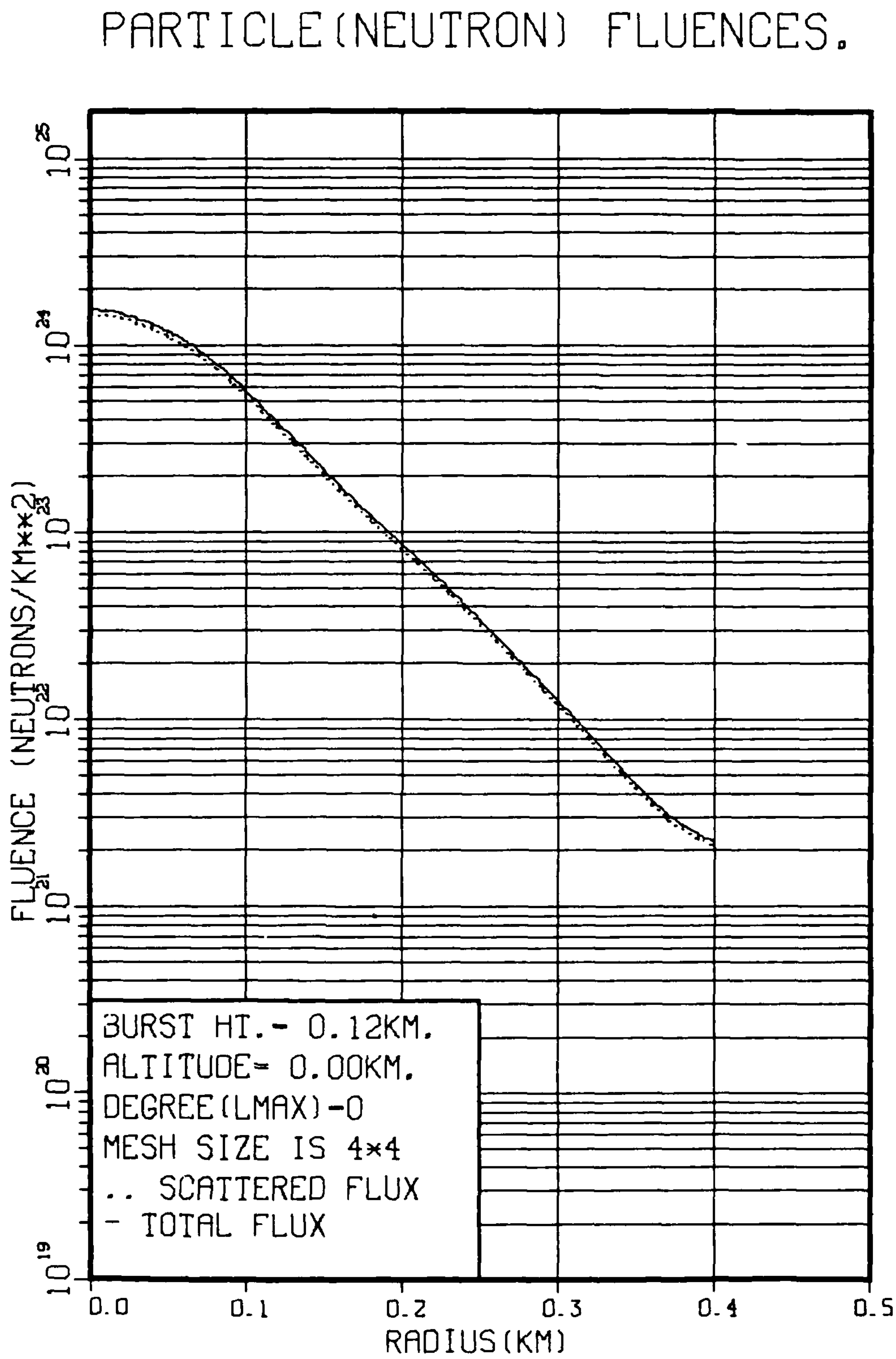

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE= 0.00KM.
DEGREE(LMAX)-0
MESH SIZE IS 4*4
.. SCATTERED FLUX
- TOTAL FLUX

Figure 20

PARTICLE(NEUTRON) FLUENCES.

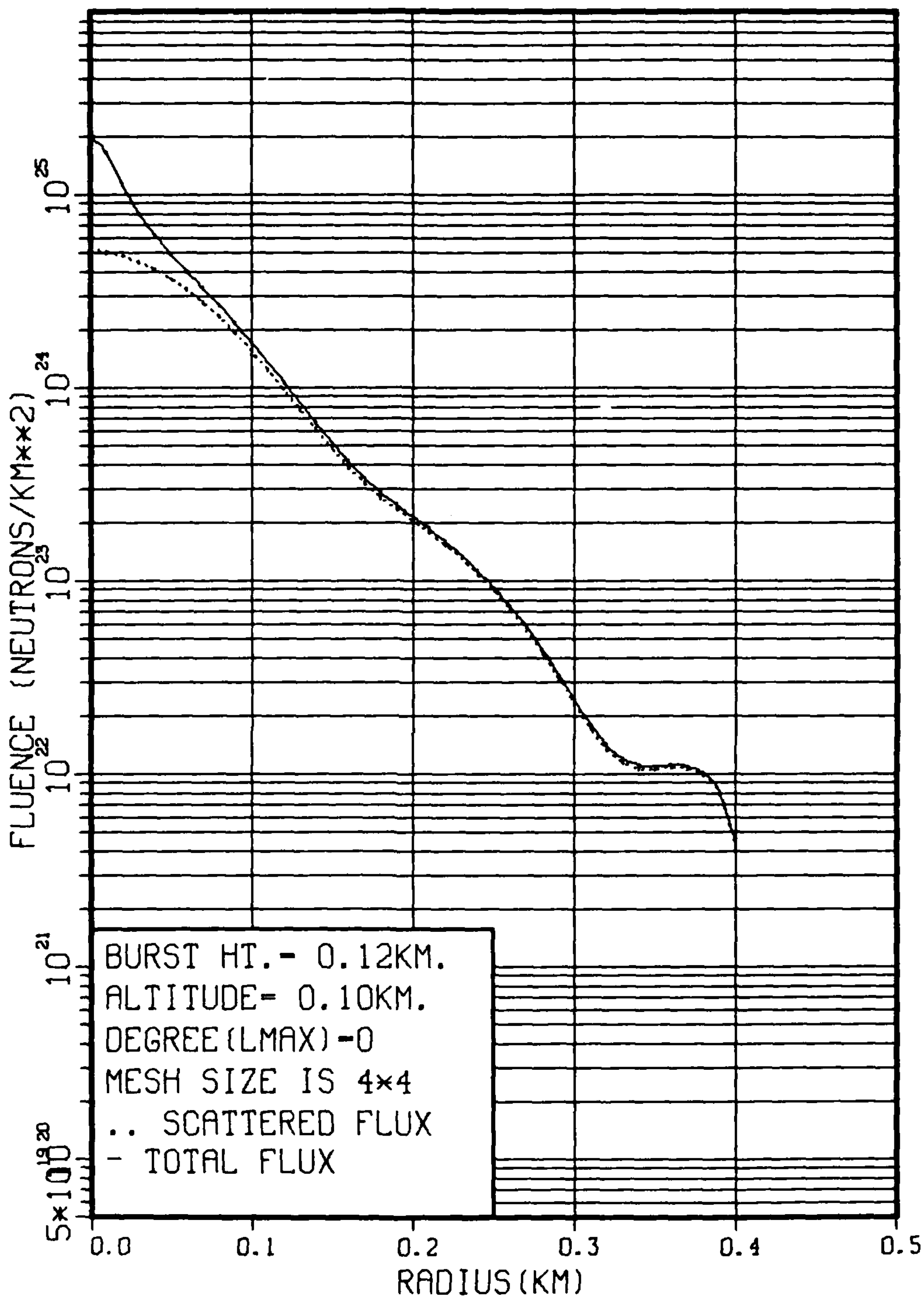


Figure 21

PARTICLE(NEUTRON) FLUENCES.

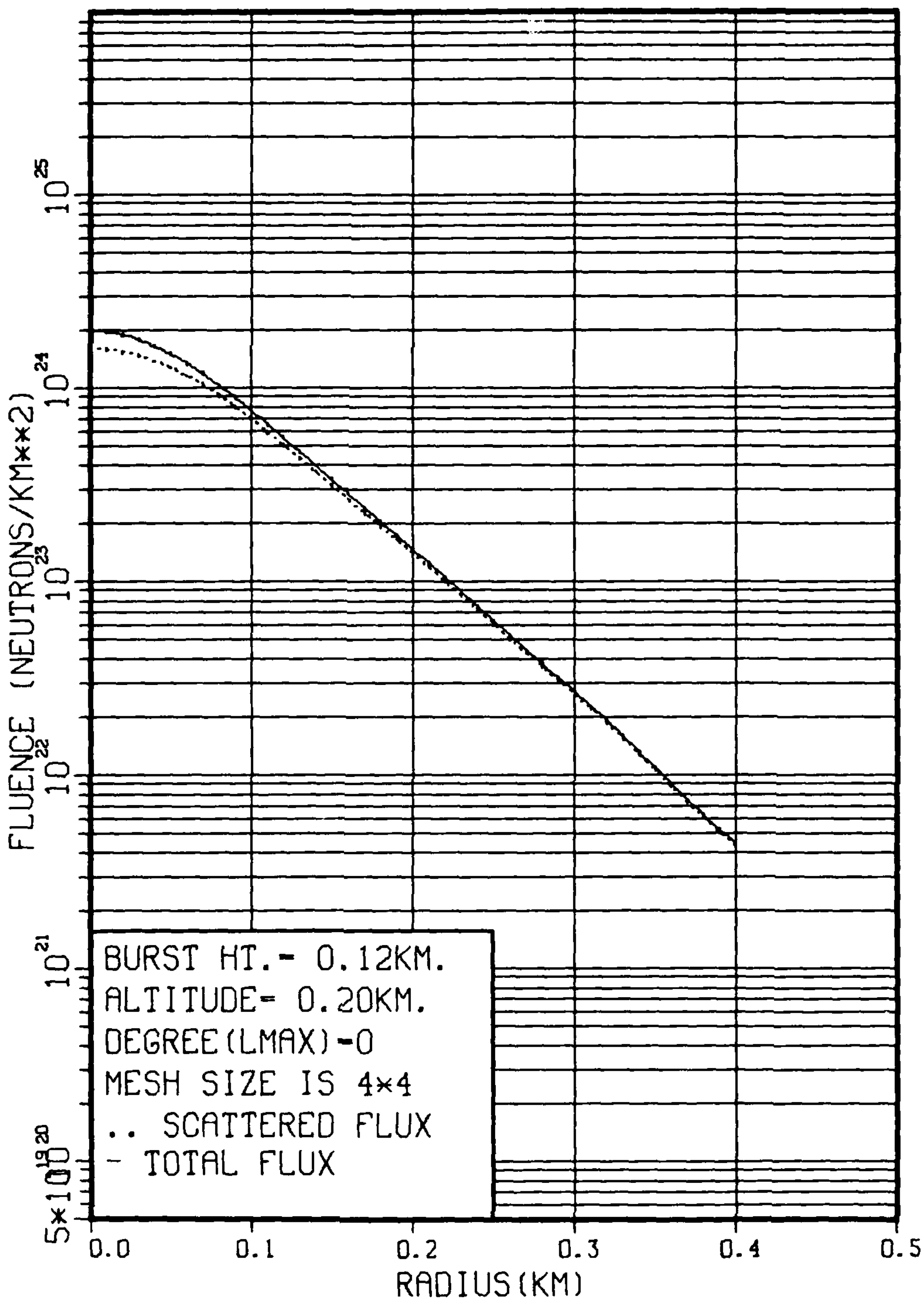


Figure 22

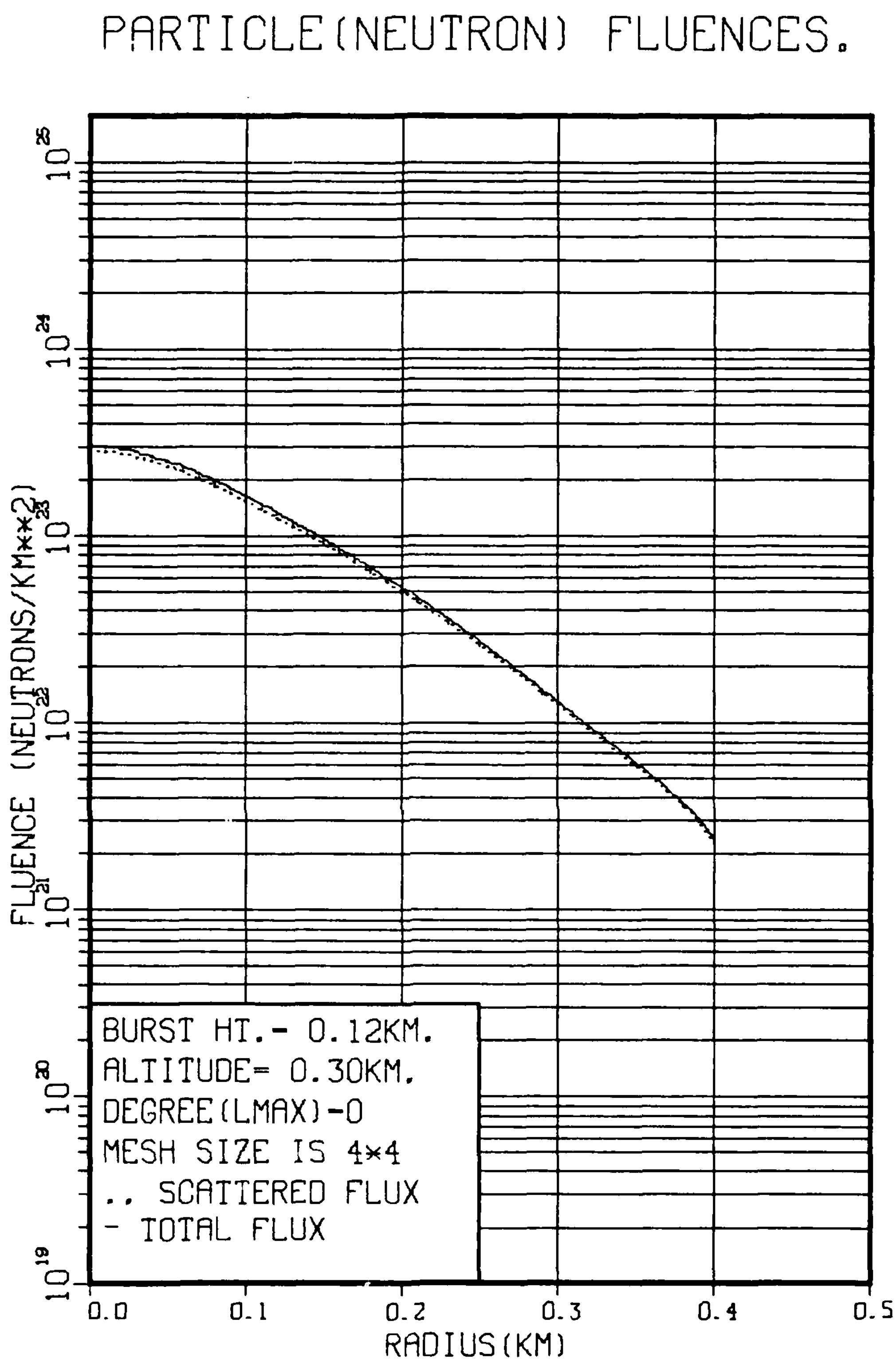

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
RADIUS(KM)
0.0
0.1
0.2
0.3
0.4
0.5
BURST HT.- 0.12KM.
ALTITUDE= 0.30KM.
DEGREE(LMAX)-0
MESH SIZE IS 4*4
.. SCATTERED FLUX
- TOTAL FLUX

Figure 23

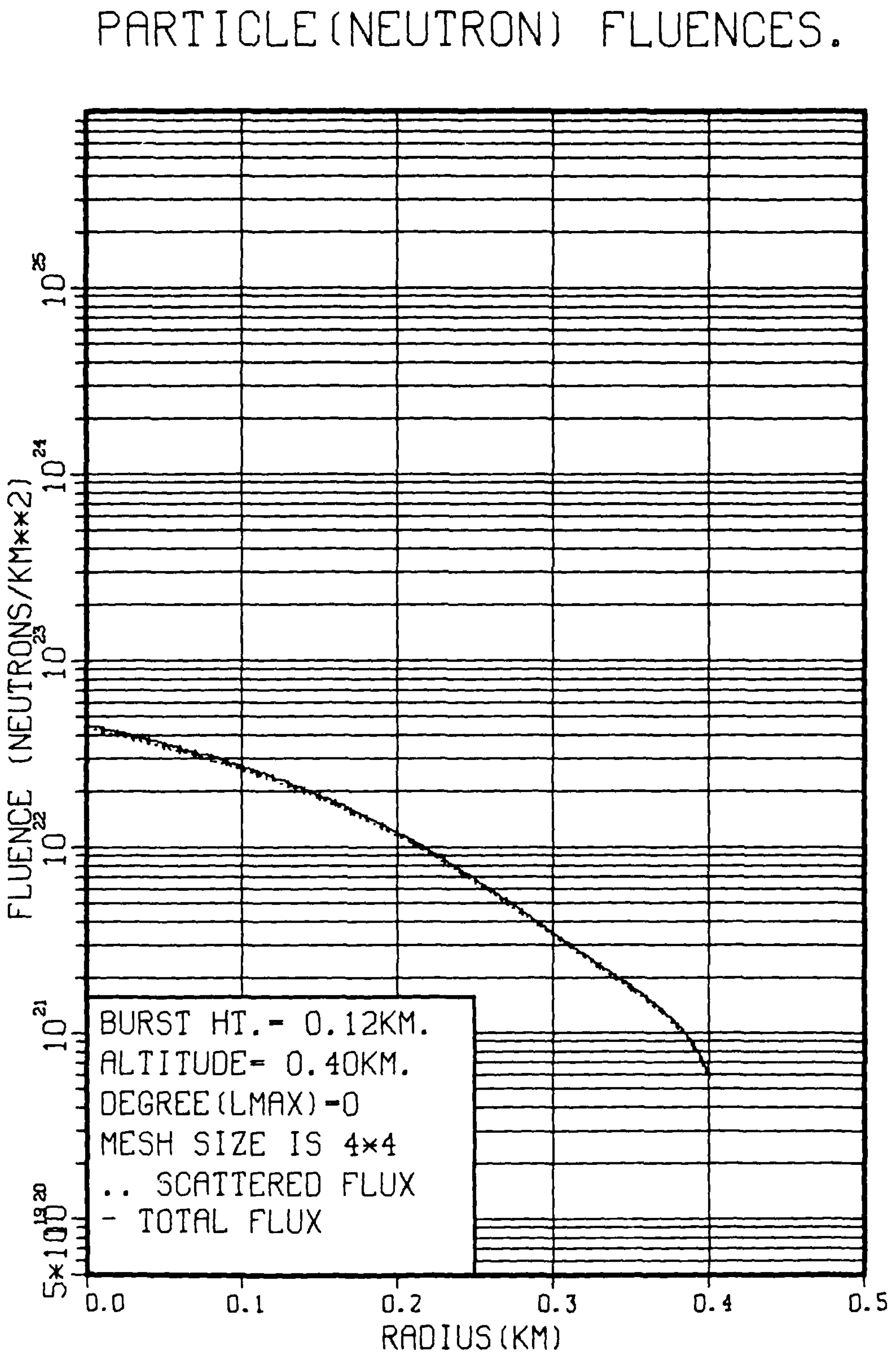

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE= 0.40KM.
DEGREE(LMAX)-0
MESH SIZE IS 4*4
.. SCATTERED FLUX
- TOTAL FLUX
0.0
0.1
0.2
0.3
0.4
0.5

Figure 24

PARTICLE(NEUTRON) FLUENCES.

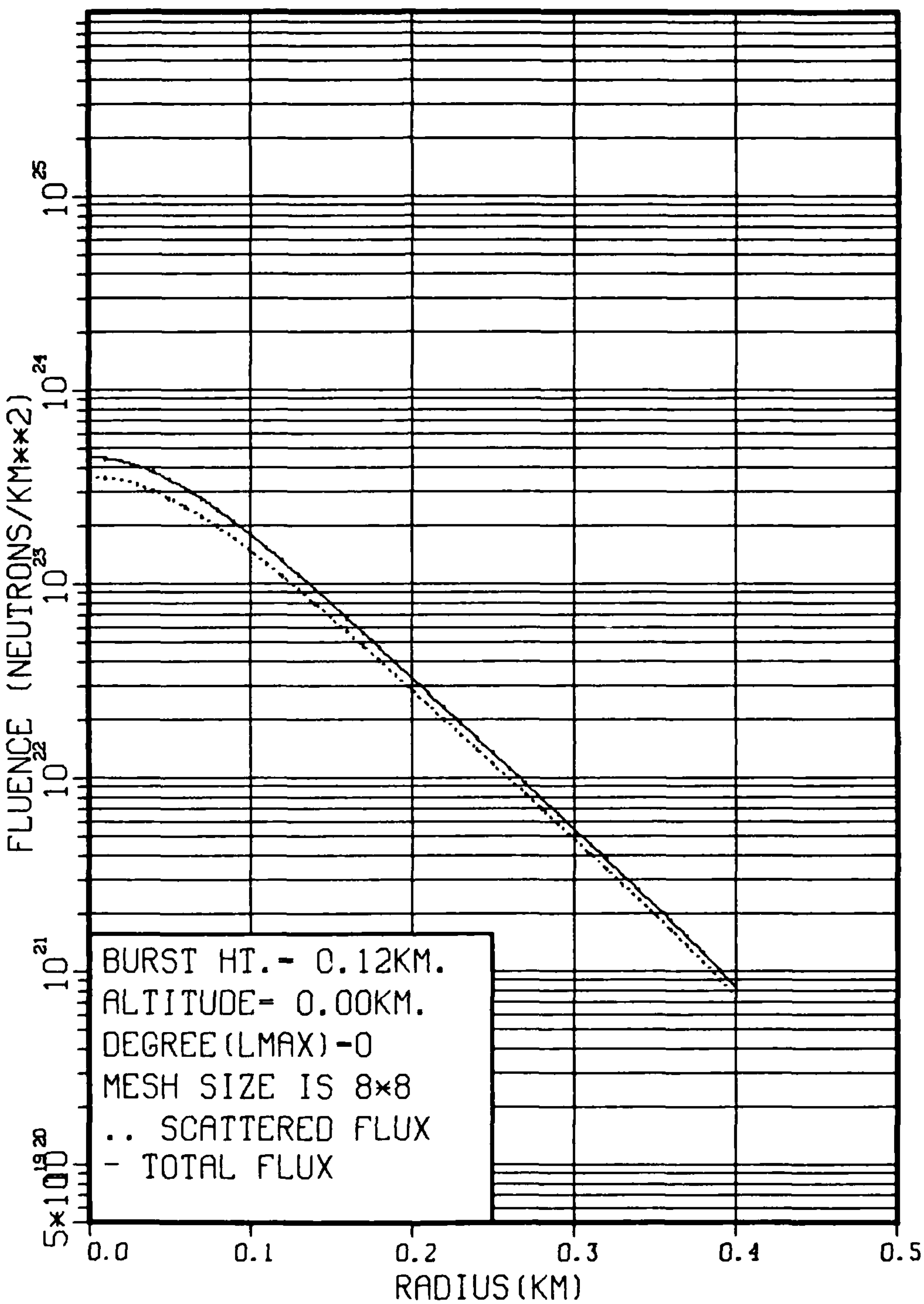


Figure 25

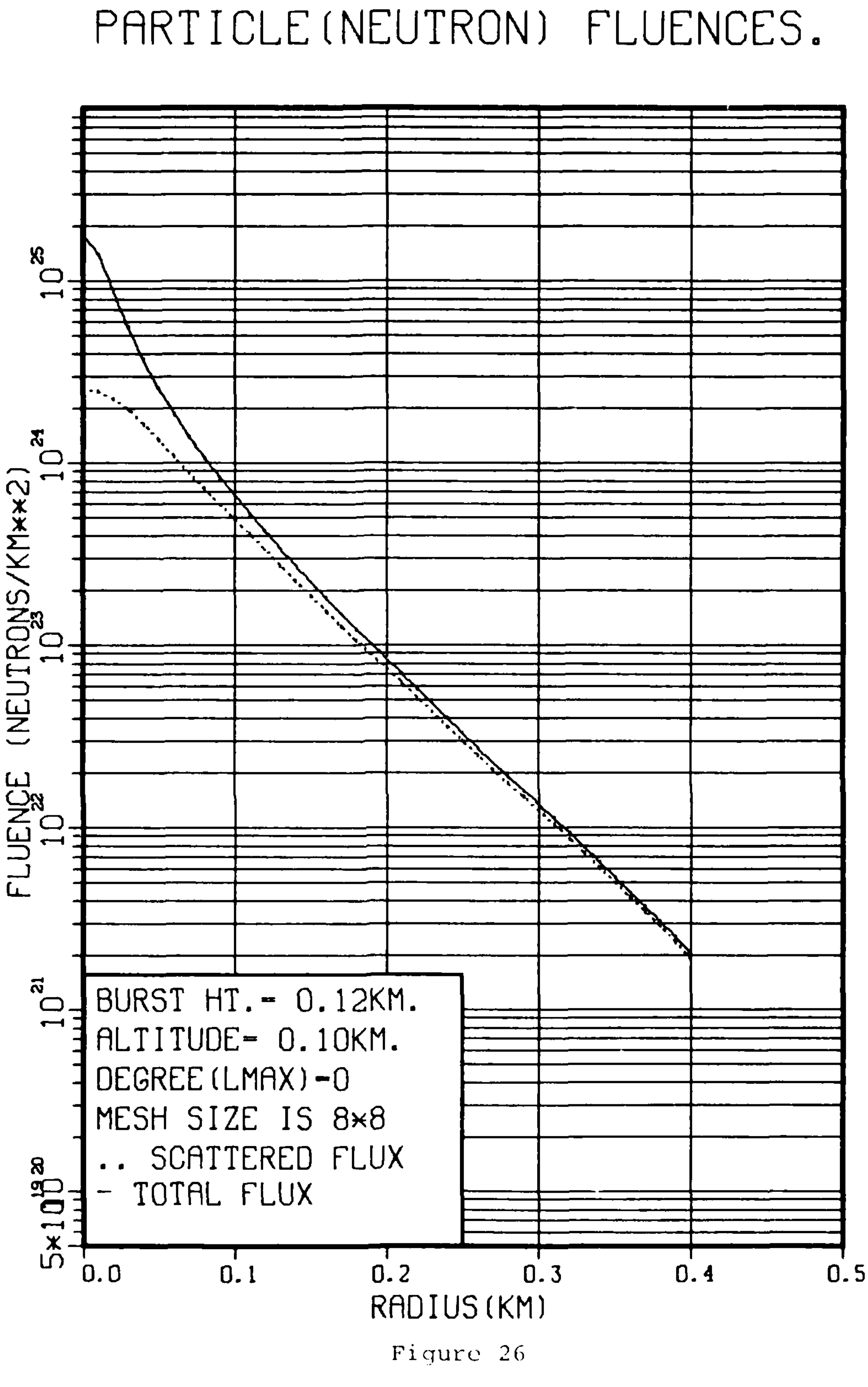

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^25
10^24
10^23
10^22
10^21
10^20
5*10^19
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.= 0.12KM.
ALTITUDE= 0.10KM.
DEGREE(LMAX)=0
MESH SIZE IS 8*8
.. SCATTERED FLUX
- TOTAL FLUX

Figure 26

PARTICLE(NEUTRON) FLUENCES.

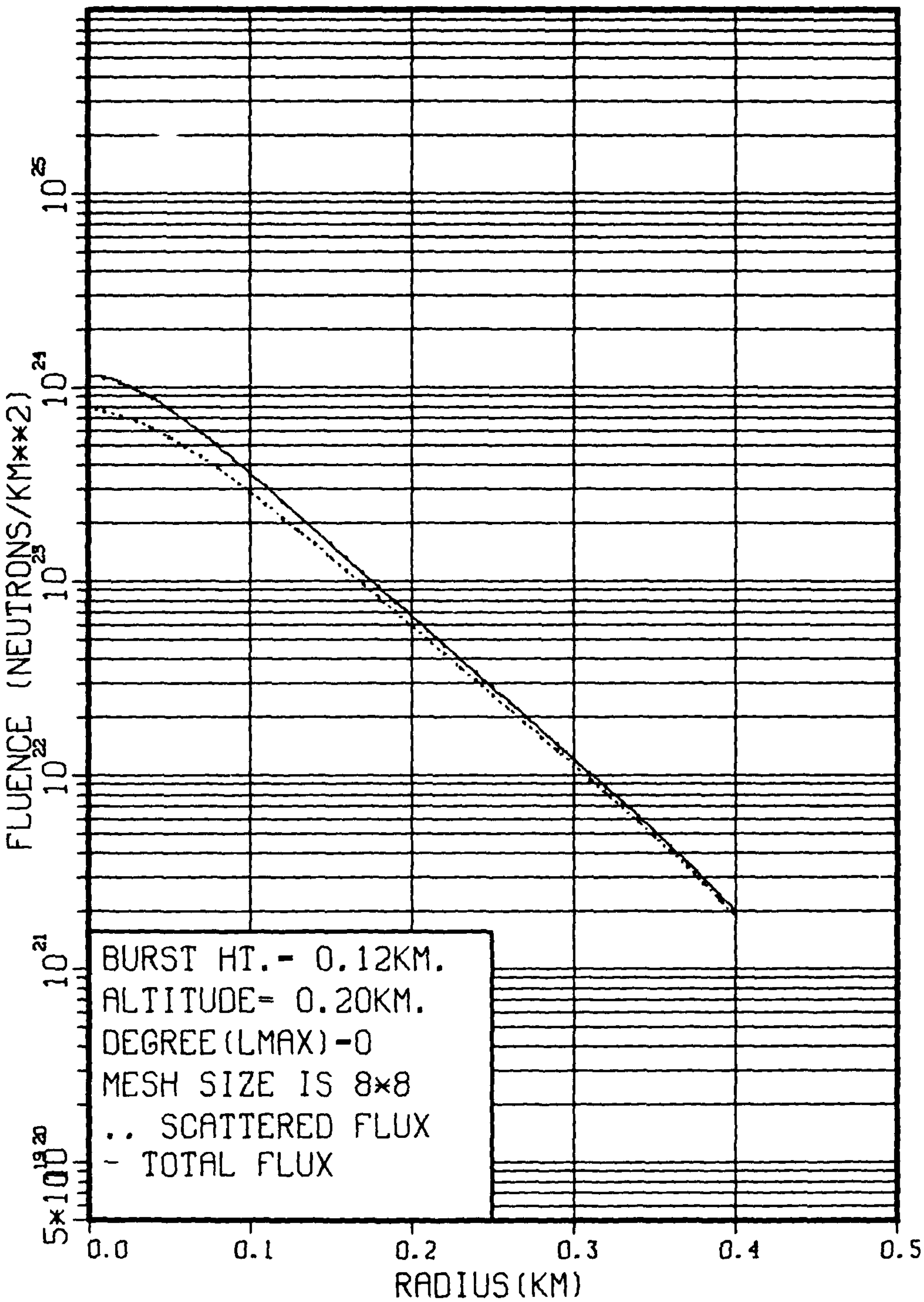
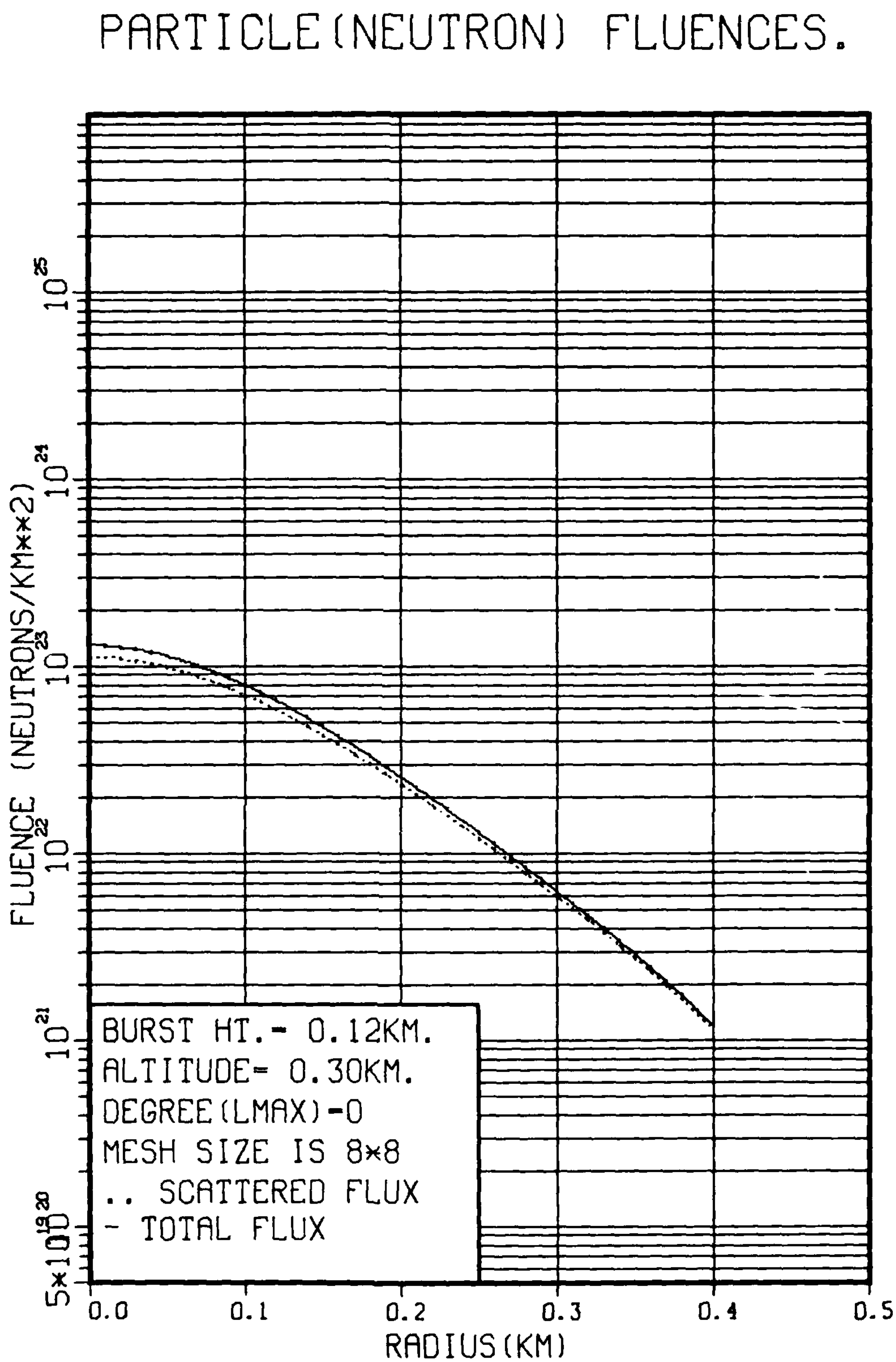


Figure 27



PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^25
10^24
10^23
10^22
10^21
5*10^20
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE= 0.30KM.
DEGREE(LMAX)-0
MESH SIZE IS 8*8
.. SCATTERED FLUX
- TOTAL FLUX

Figure 28

PARTICLE(NEUTRON) FLUENCES.

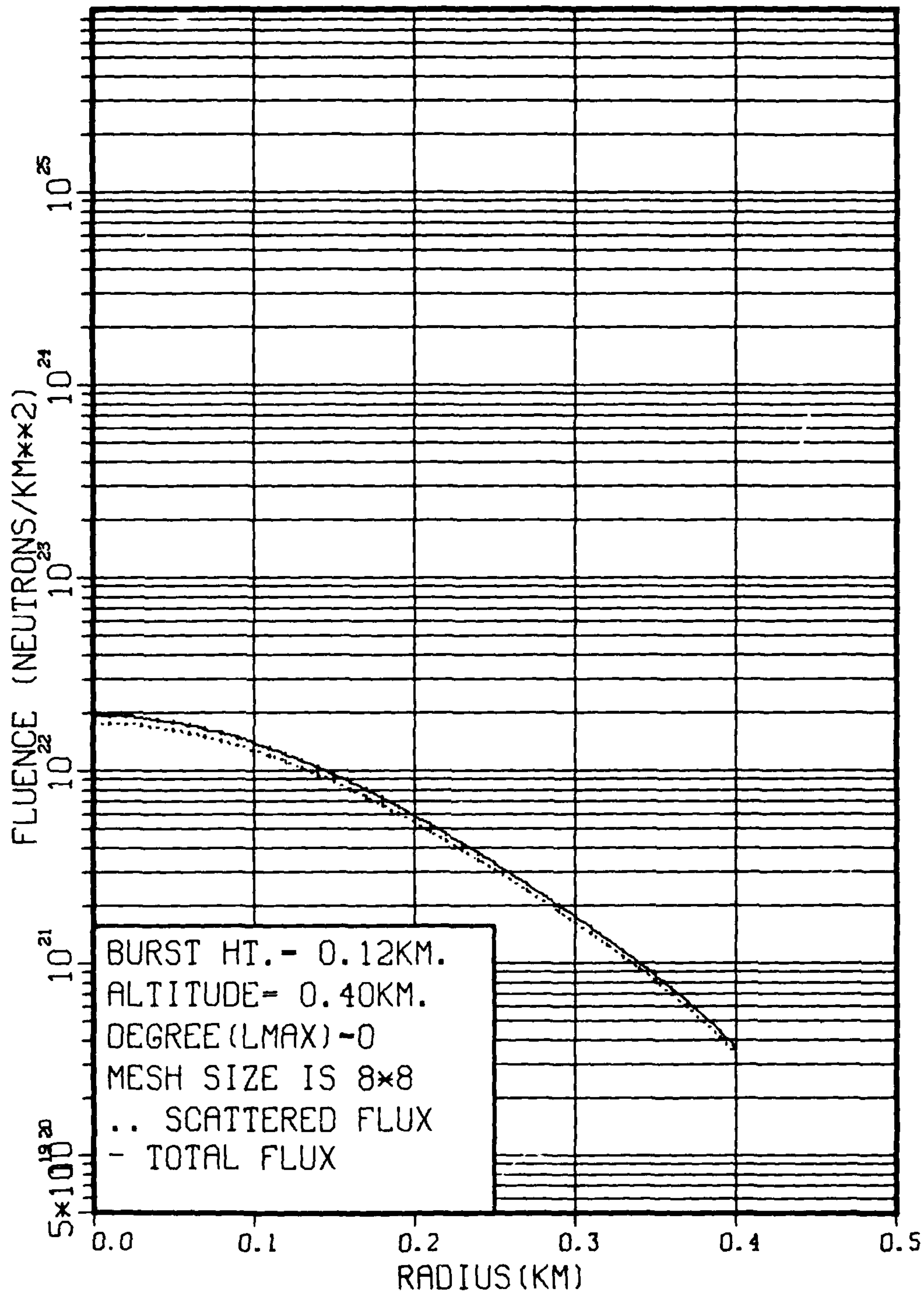
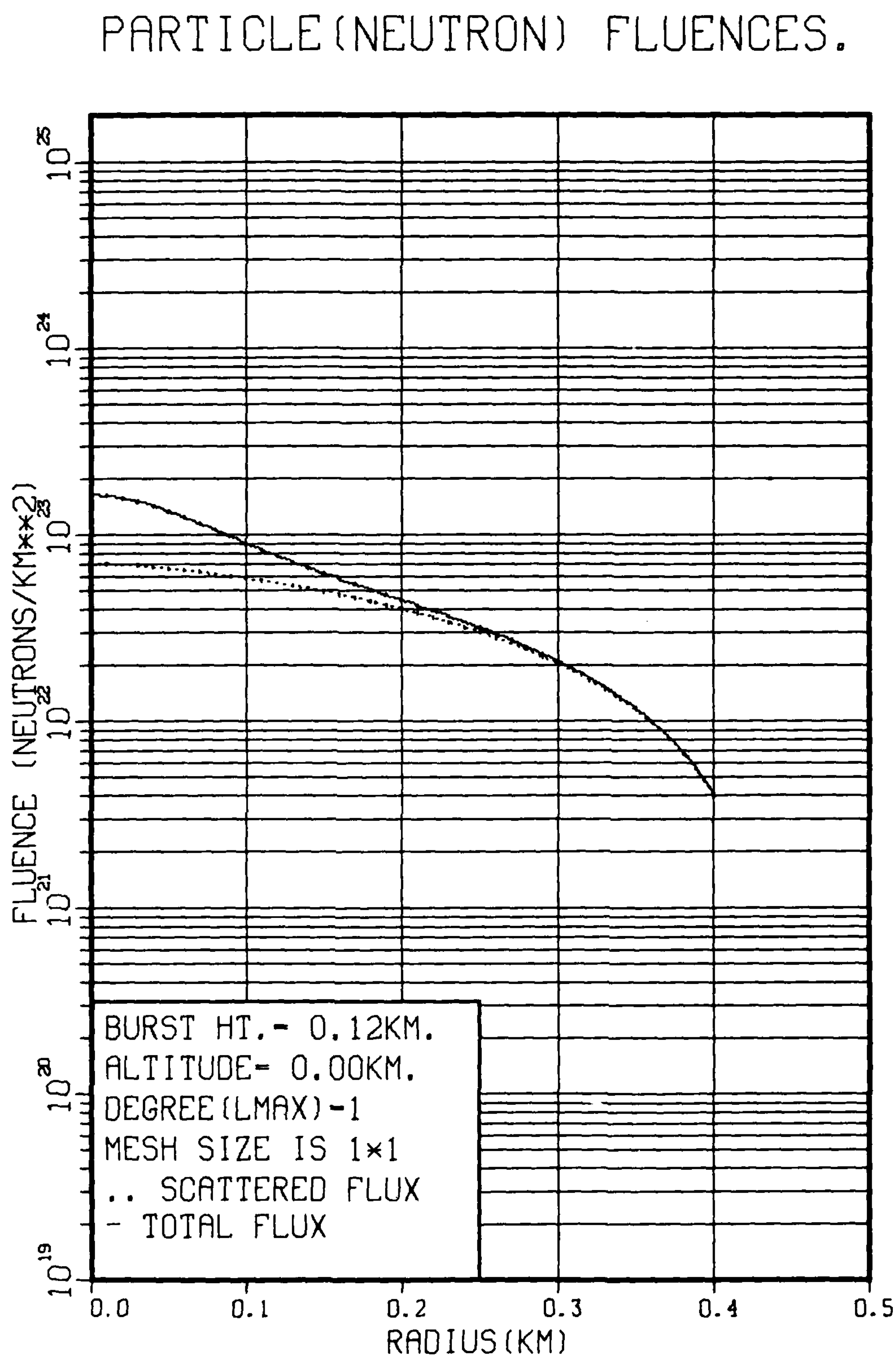
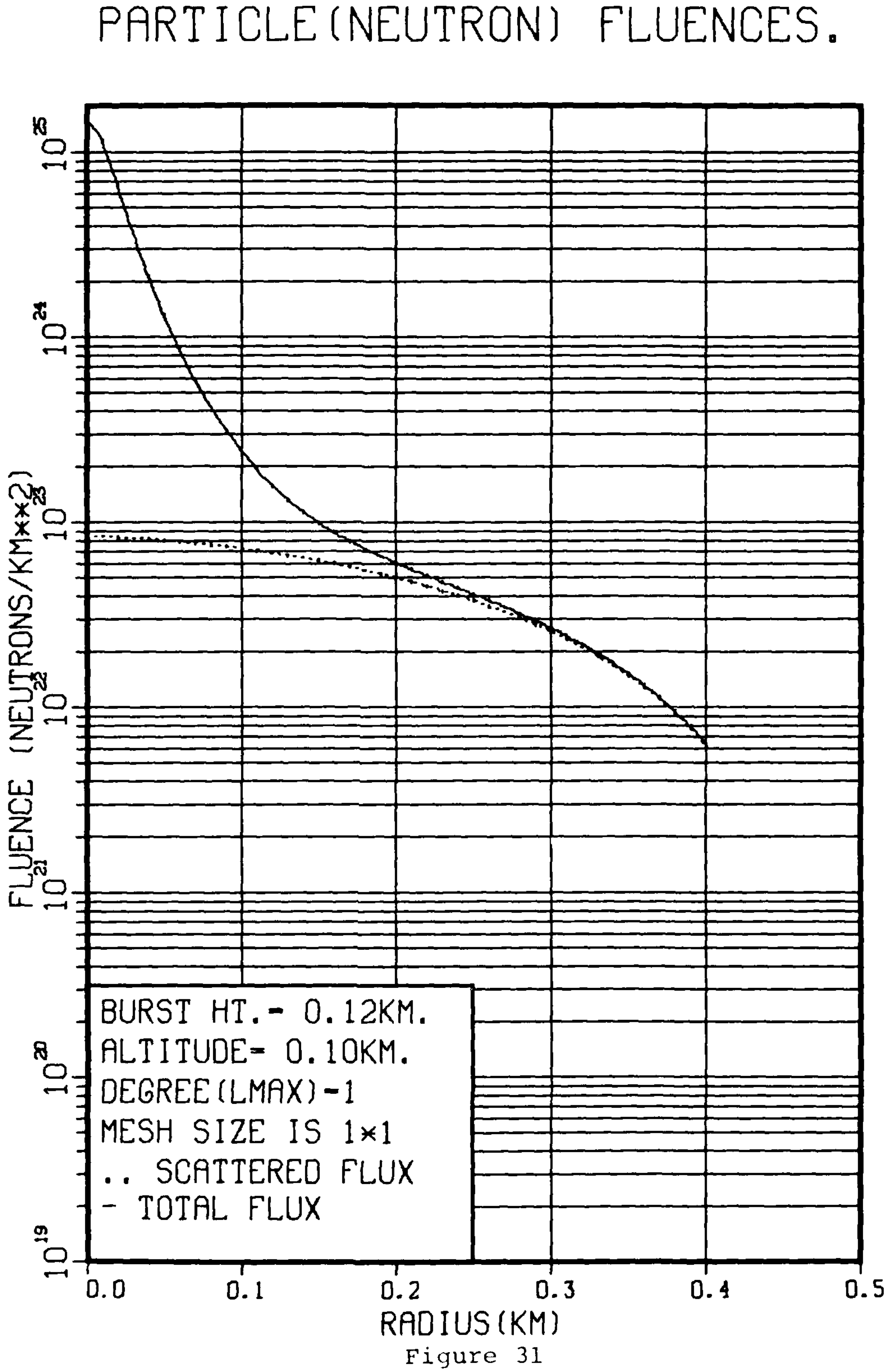


Figure 29



PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^25
10^24
10^23
10^22
10^21
10^20
10^19
BURST HT.- 0.12KM.
ALTITUDE- 0.00KM.
DEGREE(LMAX)-1
MESH SIZE IS 1*1
.. SCATTERED FLUX
- TOTAL FLUX
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)

Figure 30



PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^{25}
10^{24}
10^{23}
10^{22}
10^{21}
10^{20}
10^{19}
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.= 0.12KM.
ALTITUDE= 0.10KM.
DEGREE(LMAX)=1
MESH SIZE IS 1*1
.. SCATTERED FLUX
- TOTAL FLUX

Figure 31

PARTICLE(NEUTRON) FLUENCES.

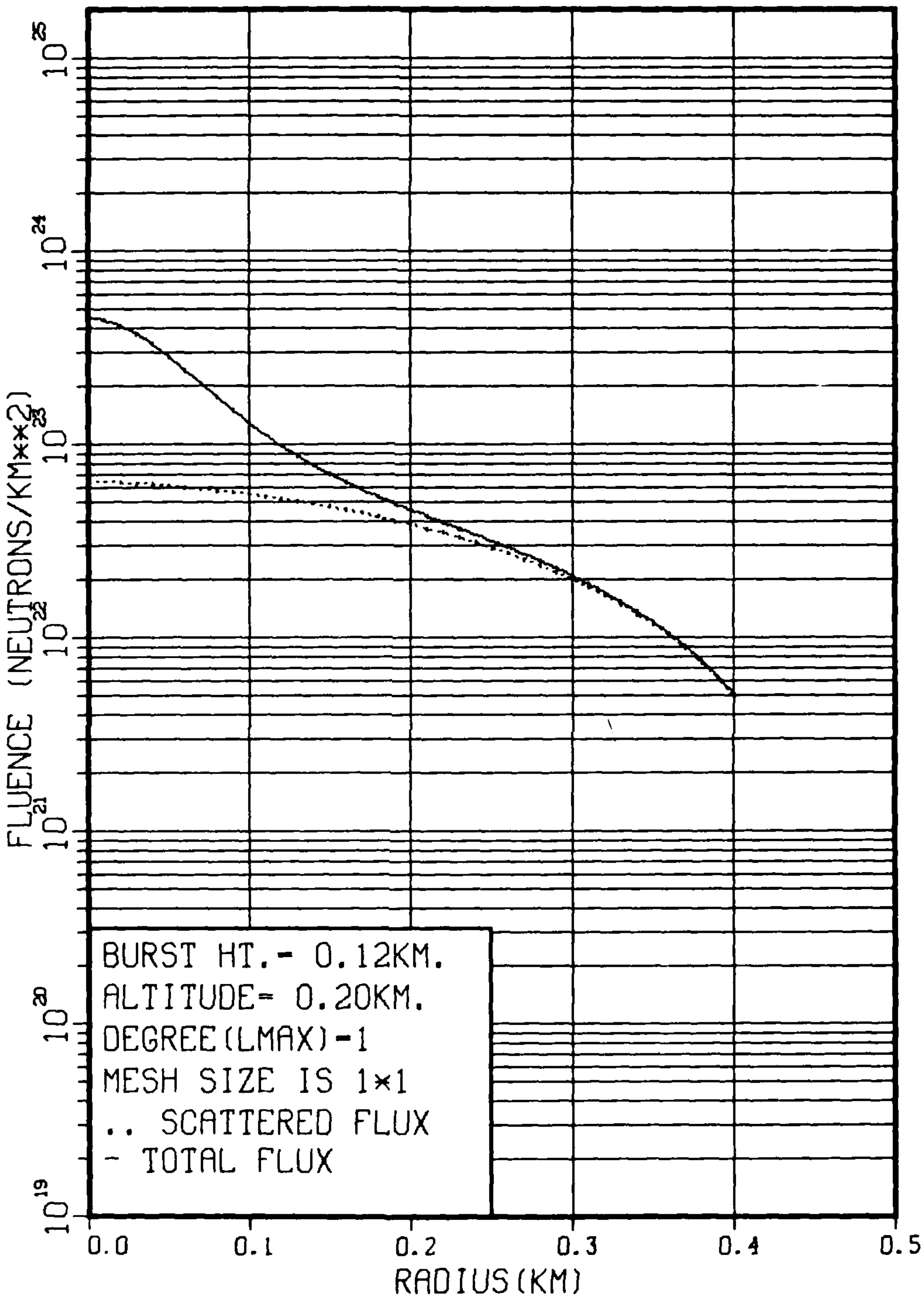


Figure 32

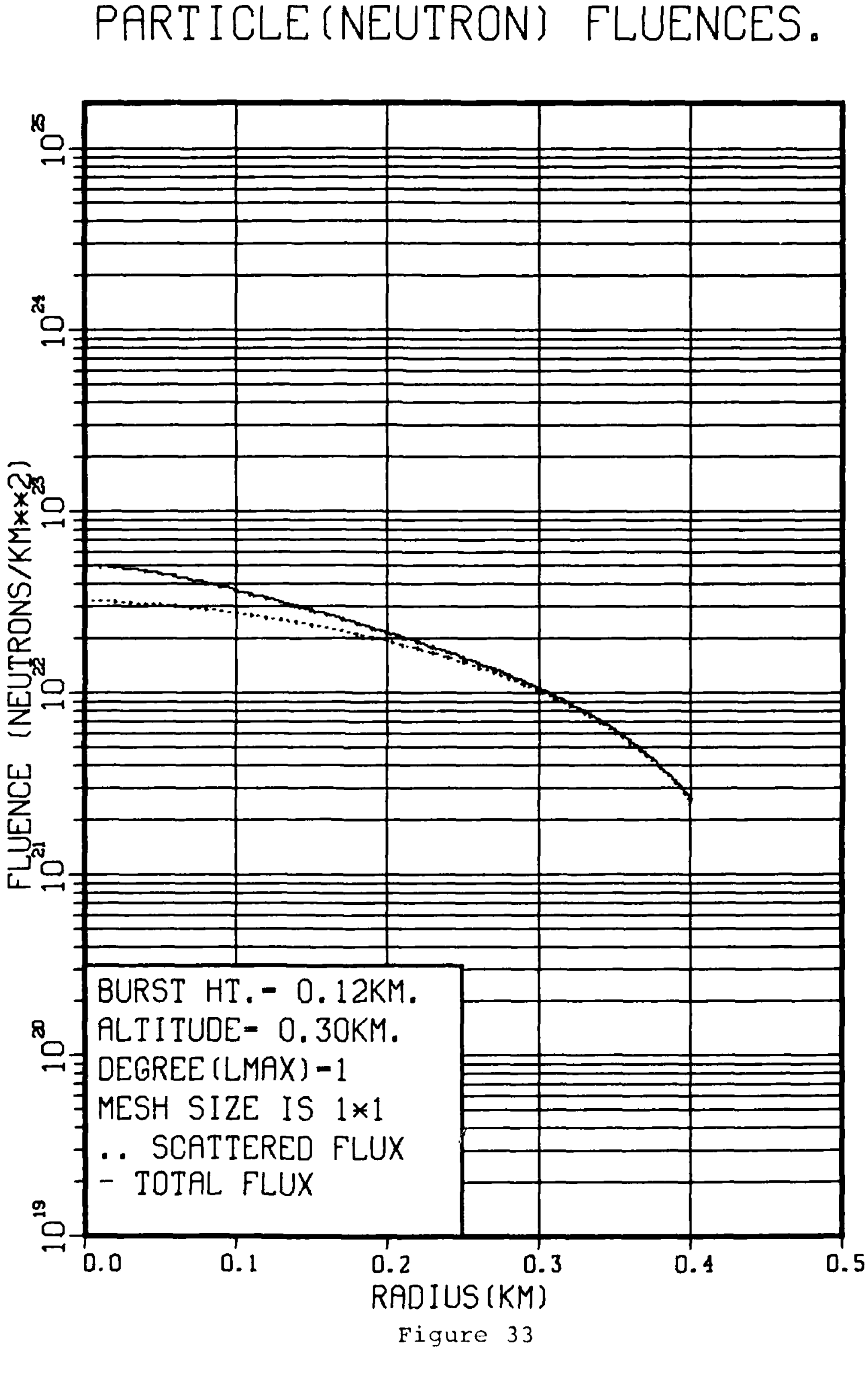

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^25
10^24
10^23
10^22
10^21
10^20
10^19
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE- 0.30KM.
DEGREE(LMAX)-1
MESH SIZE IS 1*1
.. SCATTERED FLUX
- TOTAL FLUX

Figure 33

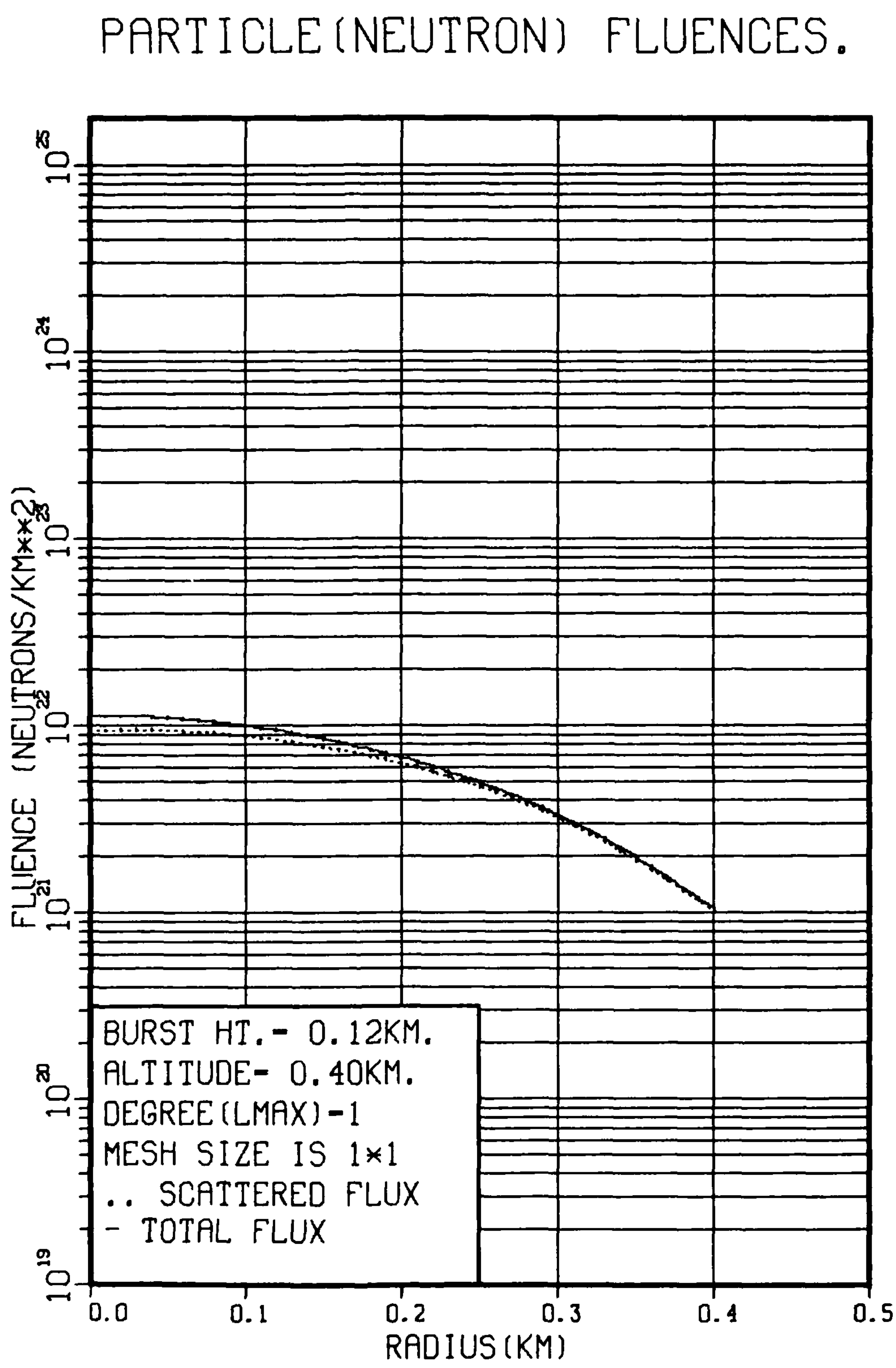

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
RADIUS(KM)
0.0
0.1
0.2
0.3
0.4
0.5
BURST HT.- 0.12KM.
ALTITUDE- 0.40KM.
DEGREE(LMAX)-1
MESH SIZE IS 1*1
.. SCATTERED FLUX
- TOTAL FLUX

Figure 34

PARTICLE(NEUTRON) FLUENCES.

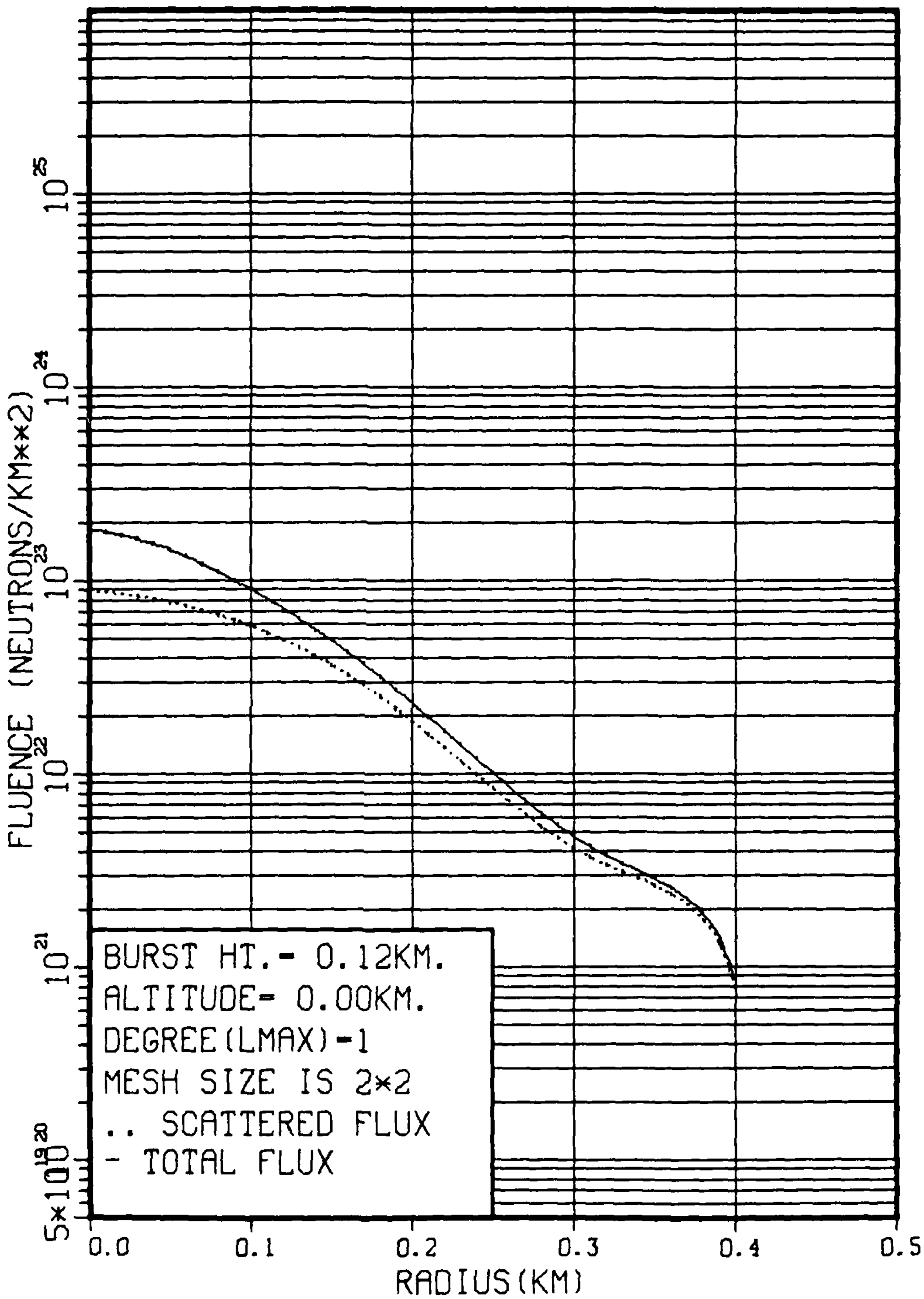


Figure 35

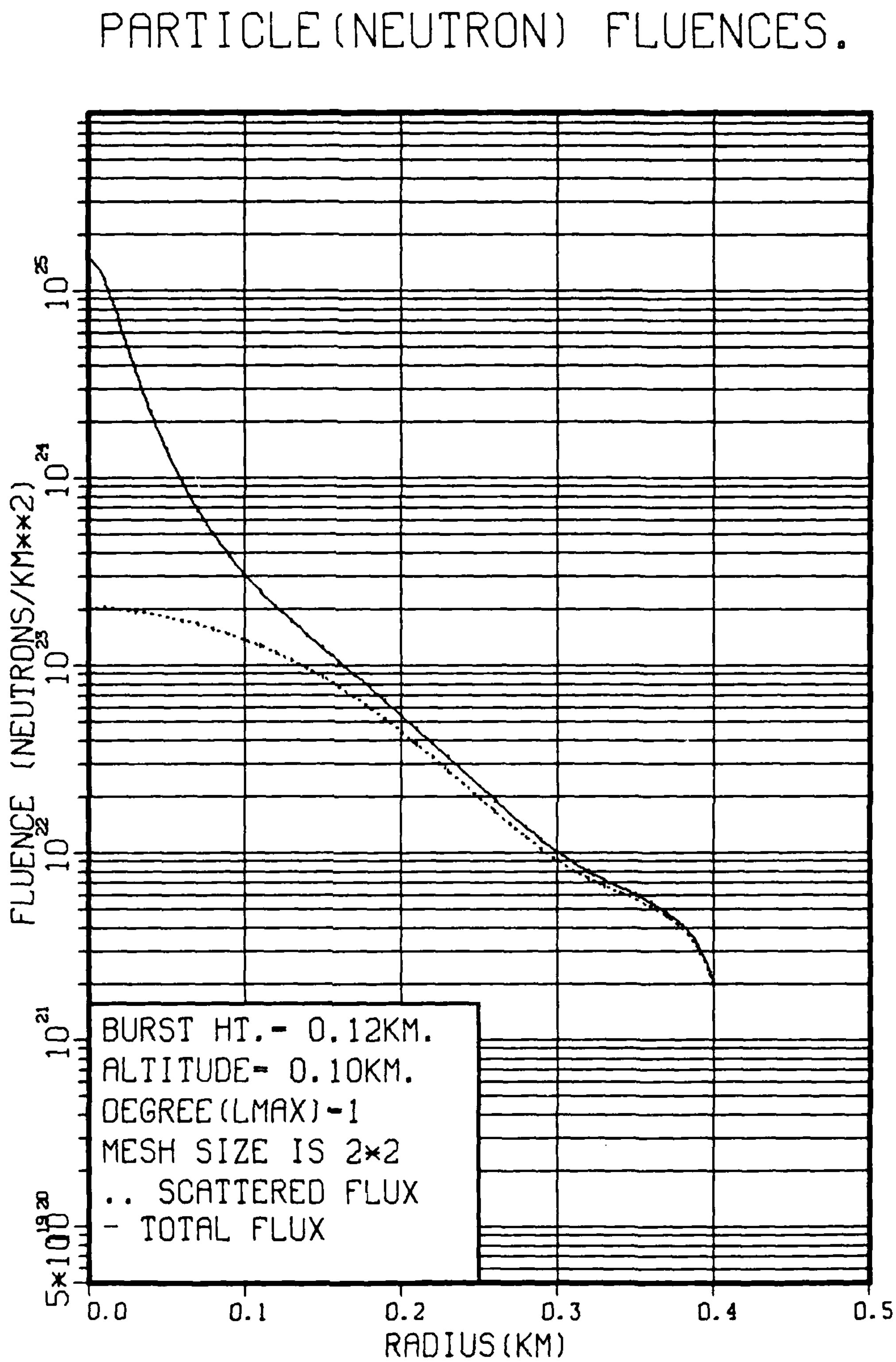

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
RADIUS(KM)
0.0
0.1
0.2
0.3
0.4
0.5
BURST HT.- 0.12KM.
ALTITUDE= 0.10KM.
DEGREE(LMAX)-1
MESH SIZE IS 2*2
.. SCATTERED FLUX
- TOTAL FLUX

Figure 36

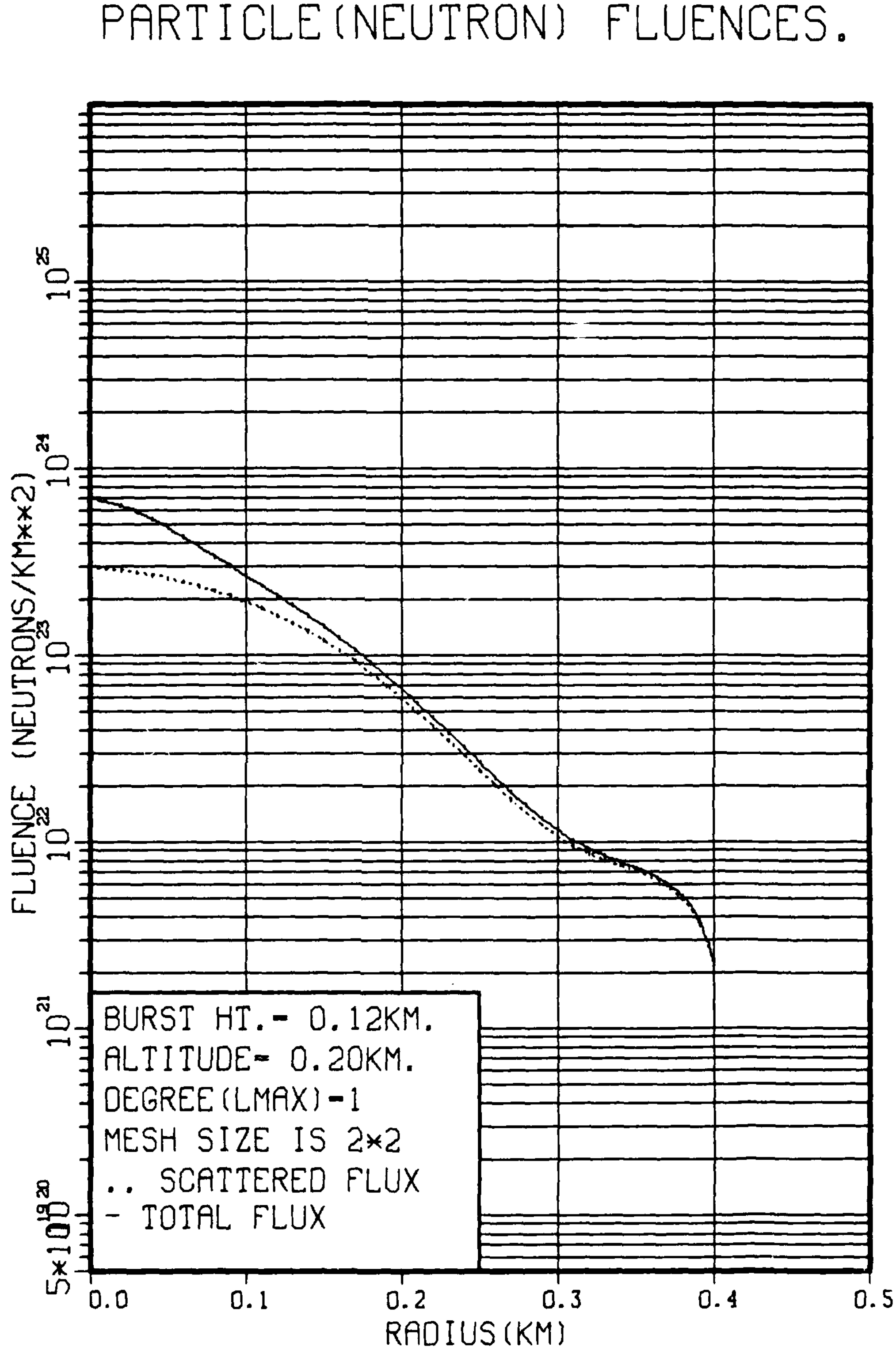

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
5*10^19
10^20
10^21
10^22
10^23
10^24
10^25
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE- 0.20KM.
DEGREE(LMAX)-1
MESH SIZE IS 2*2
.. SCATTERED FLUX
- TOTAL FLUX

Figure 37

PARTICLE(NEUTRON) FLUENCES.

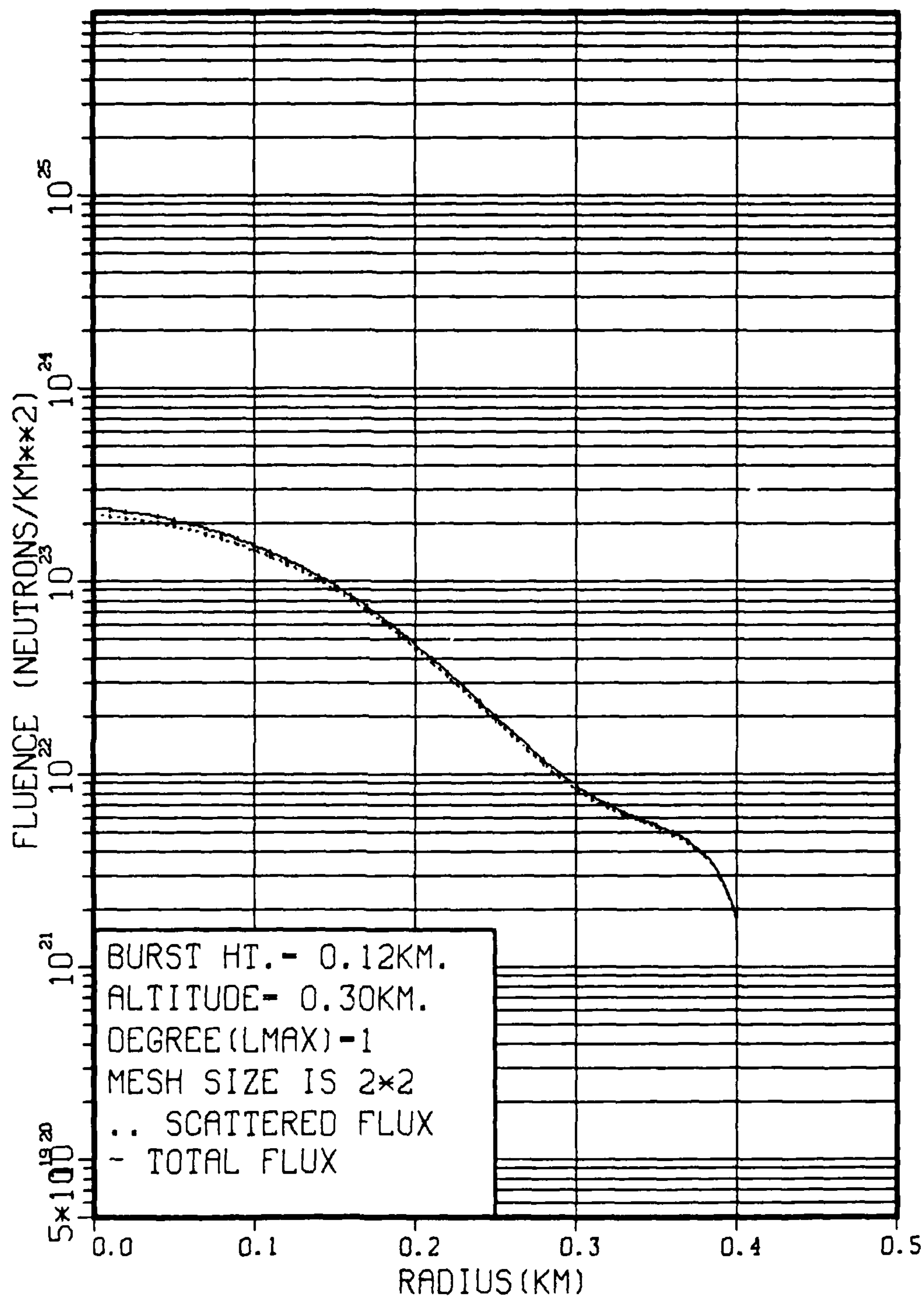


Figure 38

PARTICLE(NEUTRON) FLUENCES.

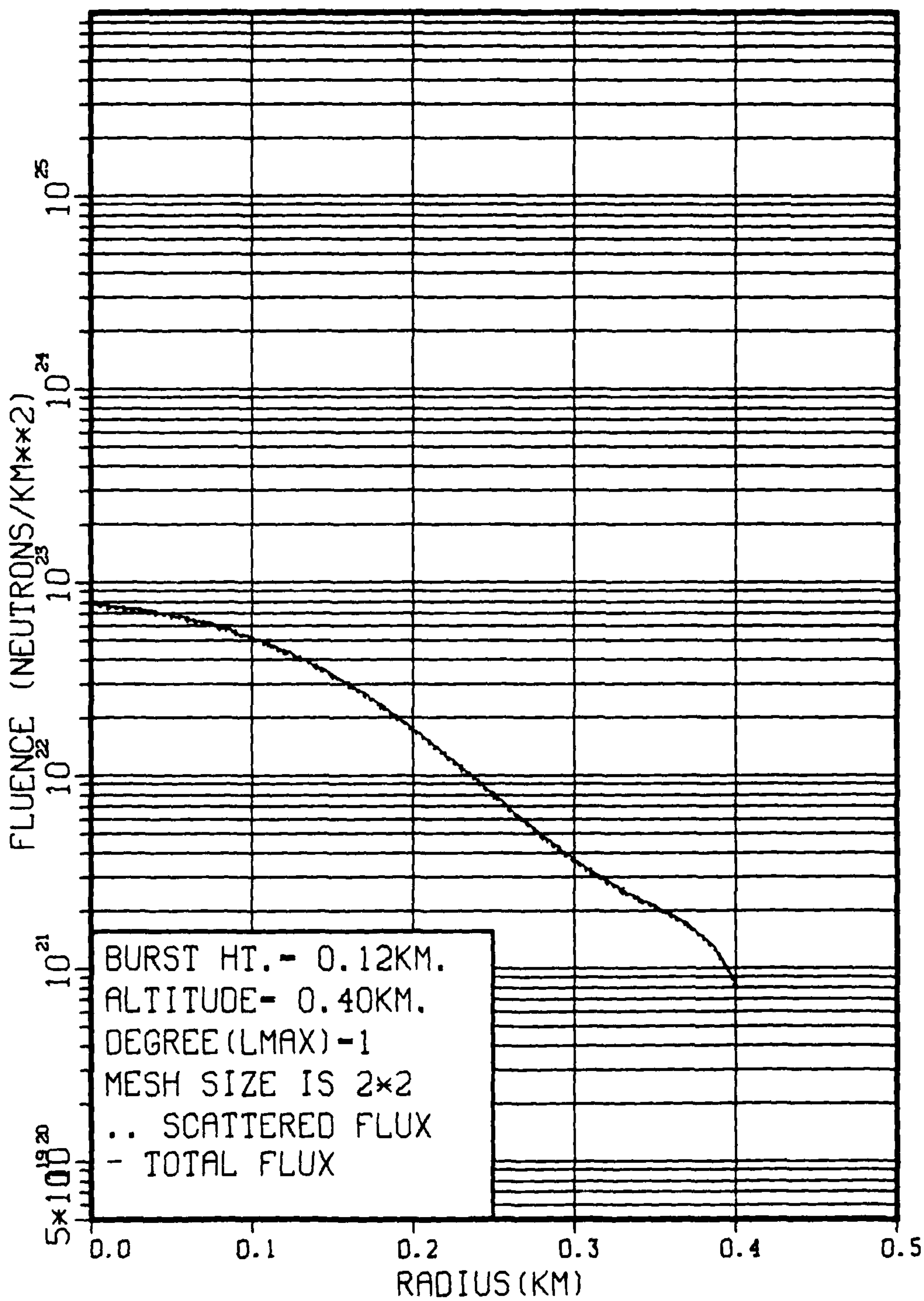


Figure 39

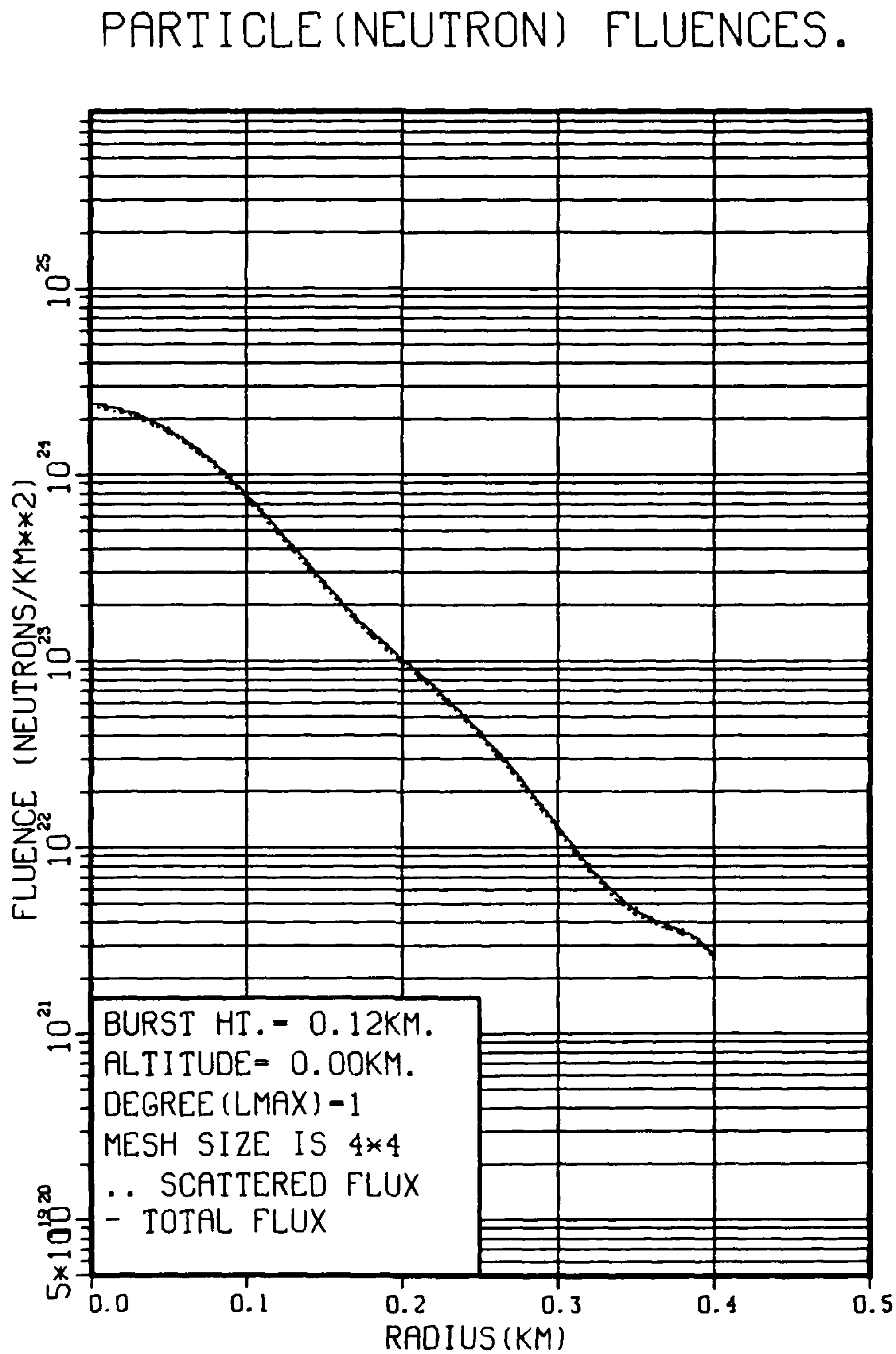
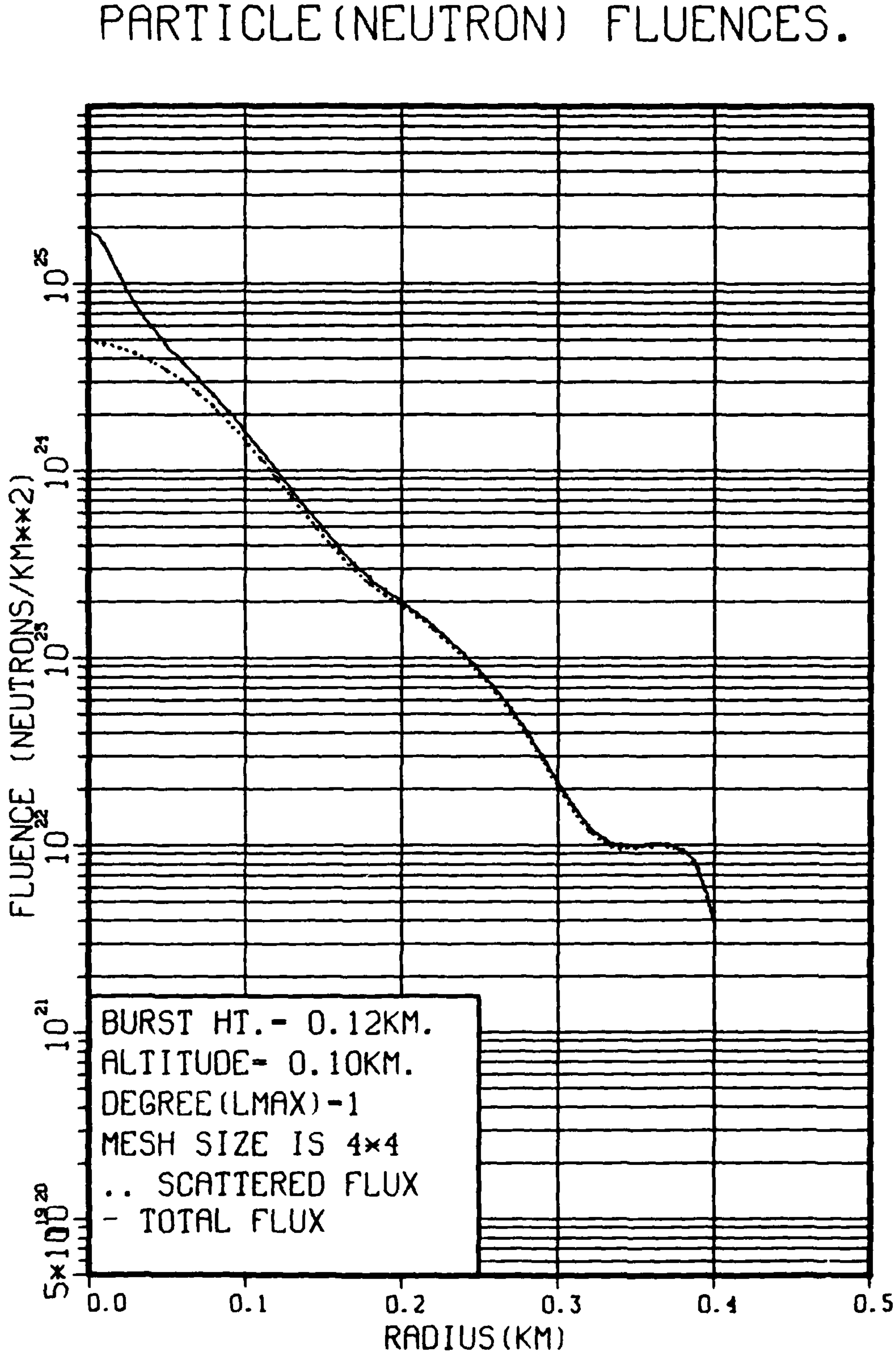

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^25
10^24
10^23
10^22
10^21
10^20
5*10^19
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.= 0.12KM.
ALTITUDE= 0.00KM.
DEGREE(LMAX)=1
MESH SIZE IS 4*4
.. SCATTERED FLUX
- TOTAL FLUX

Figure 40



PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^{25}
10^{24}
10^{23}
10^{22}
10^{21}
10^{20}
5×10^{19}
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE= 0.10KM.
DEGREE(LMAX)-1
MESH SIZE IS 4x4
.. SCATTERED FLUX
- TOTAL FLUX

Figure 41

PARTICLE(NEUTRON) FLUENCES.

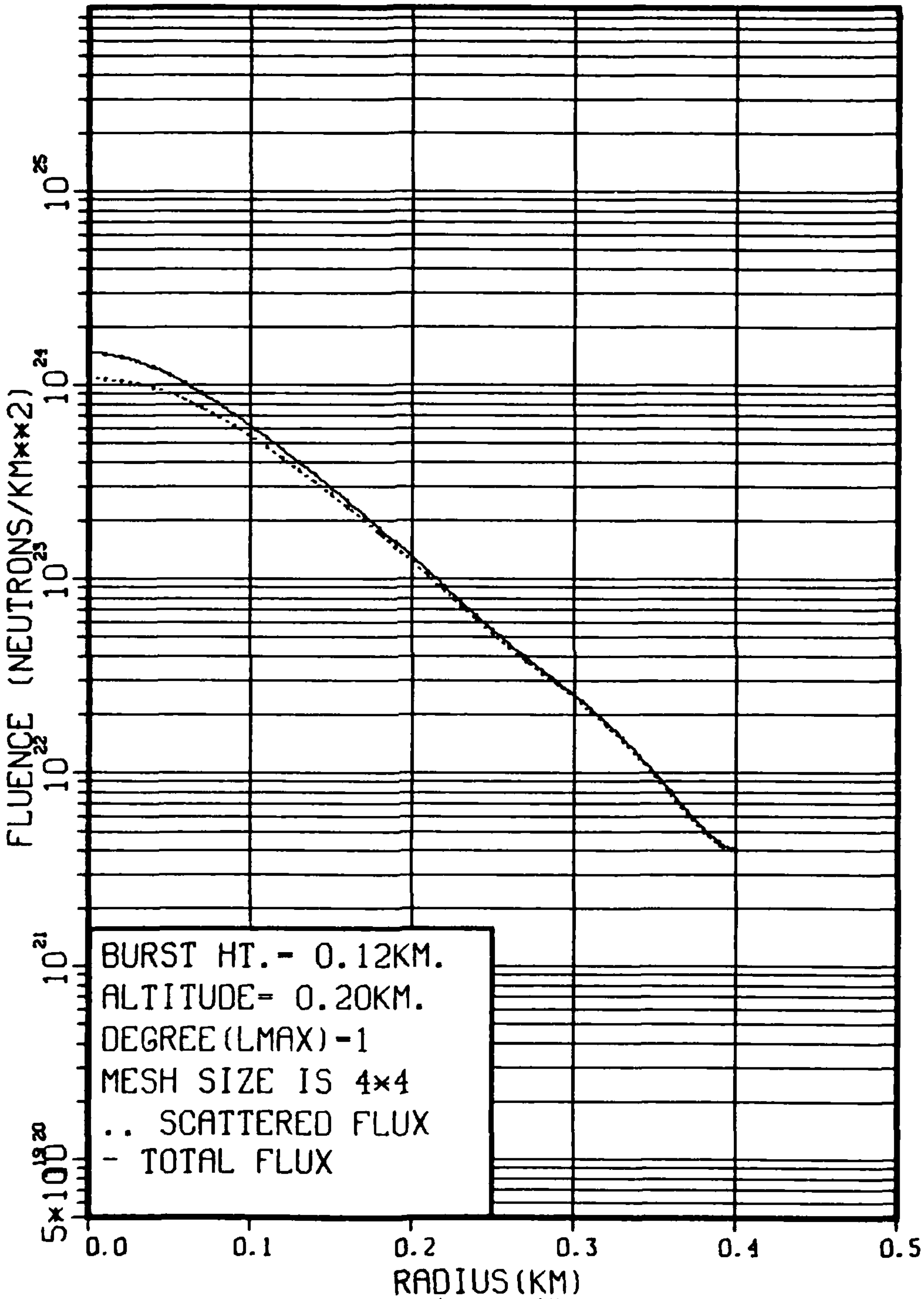
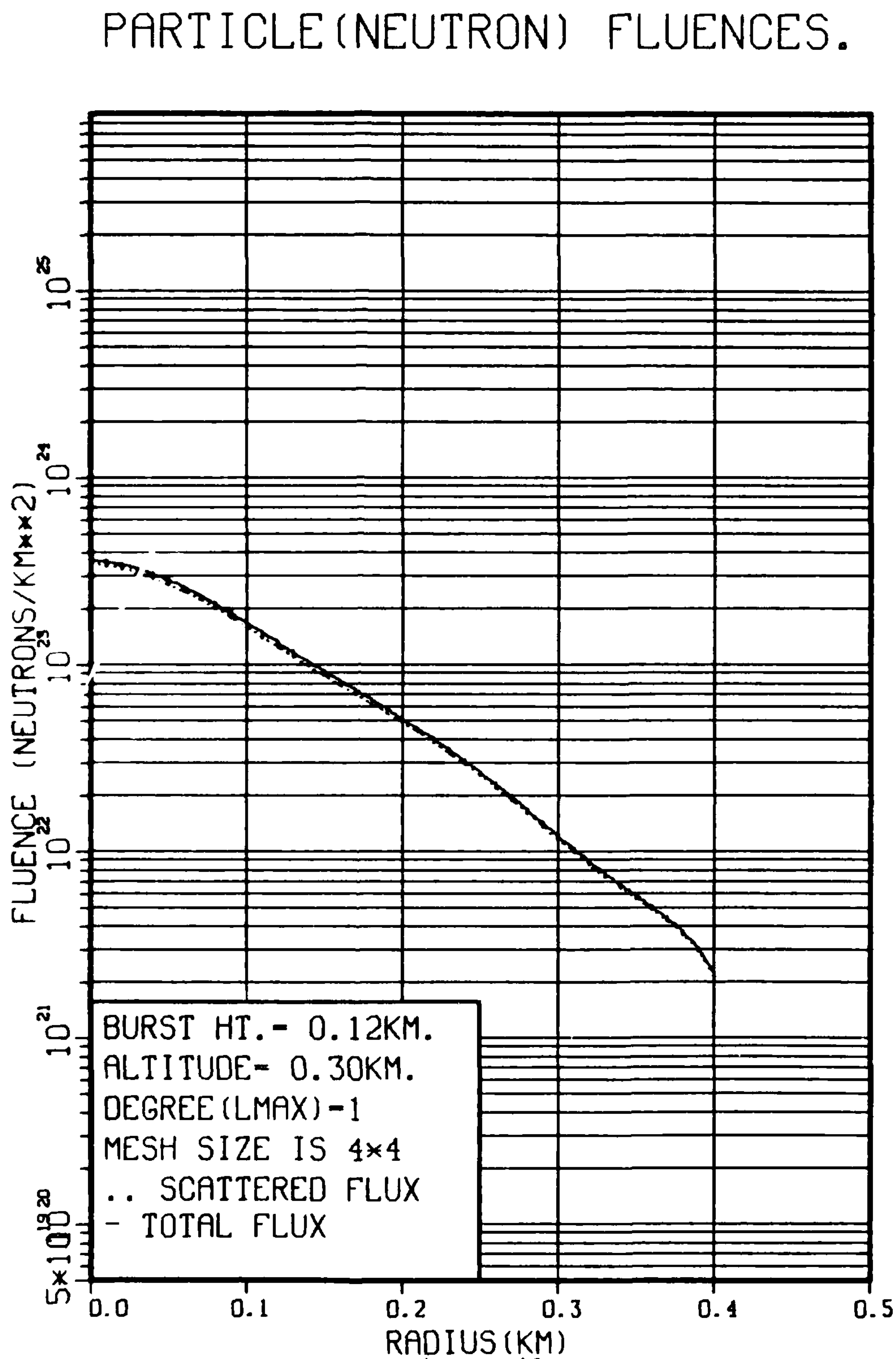


Figure 42


PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^25
10^24
10^23
10^22
10^21
5*10^19 10^20
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.- 0.12KM.
ALTITUDE- 0.30KM.
DEGREE(LMAX)-1
MESH SIZE IS 4*4
.. SCATTERED FLUX
- TOTAL FLUX
Figure 43

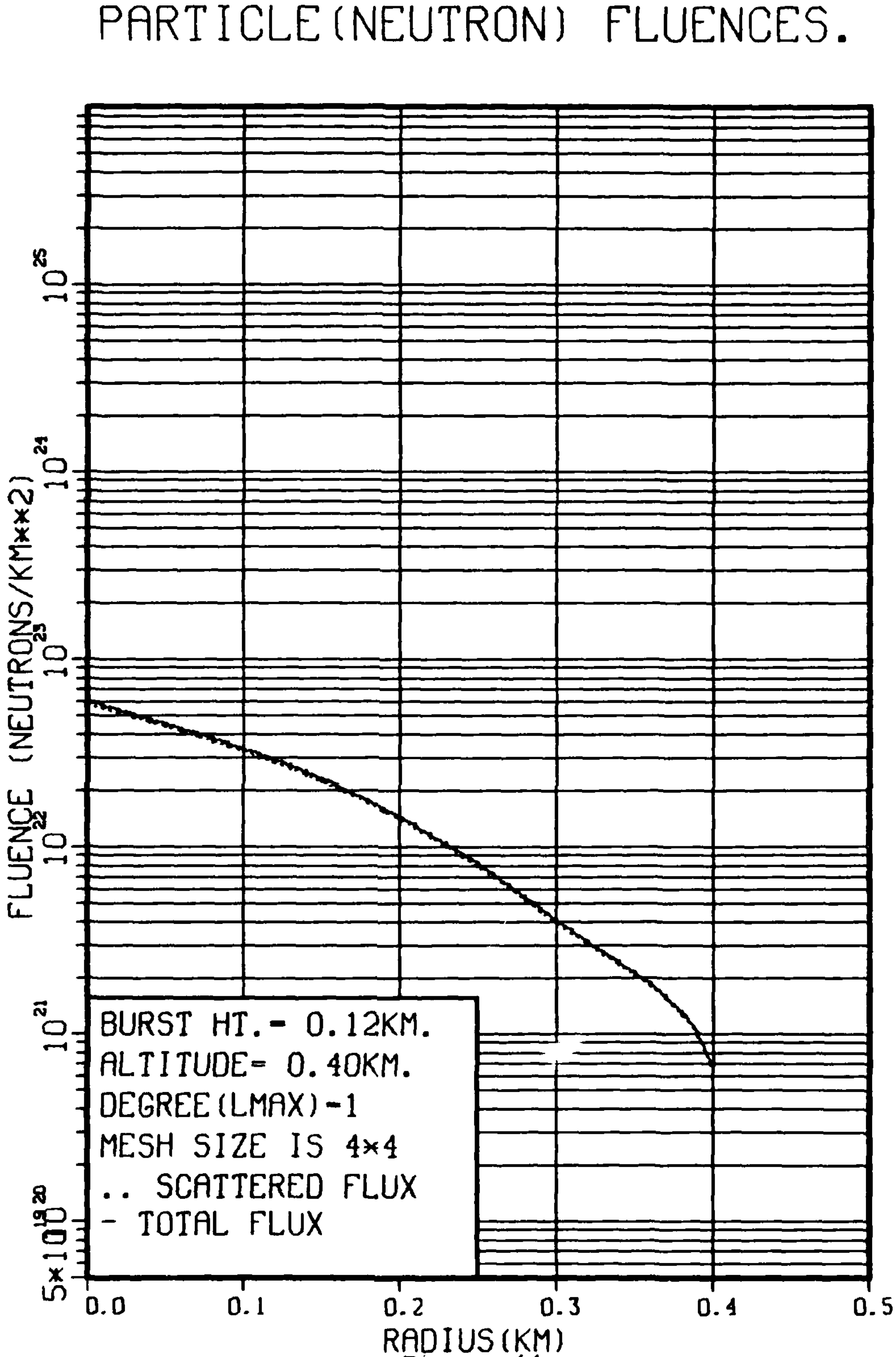

PARTICLE(NEUTRON) FLUENCES.
FLUENCE (NEUTRONS/KM**2)
10^25
10^24
10^23
10^22
10^21
10^20
5*10^19
0.0
0.1
0.2
0.3
0.4
0.5
RADIUS(KM)
BURST HT.= 0.12KM.
ALTITUDE= 0.40KM.
DEGREE(LMAX)=1
MESH SIZE IS 4*4
.. SCATTERED FLUX
- TOTAL FLUX

Figure 44

Vita

Eze E. Wills was born in Guyana, South America, in April, 1951. He served as a Food Inspection Specialist in the enlisted ranks of the U.S. Army from 1972 to 1974. In 1974, he was promoted to the rank of Sergeant. Upon completion of his two year military commitment he was discharged from the Army in 1974. He then worked as a Security Guard with the Department of Navy, Navy Headquarters, Washington, D.C. from 1974 to 1976. In 1975 he enrolled at the University of Maryland, from which he graduated in December 1978 with the degree of Bachelor of Science, Nuclear-Chemical Engineering. He also completed ROTC training at the University of Maryland and was commissioned to the USAF in December 1978. He subsequently attended Graduate School at the University of Maryland and worked as a Chemical Engineer with the Department of the Navy, Naval Ordinance Station, Indian Head, Maryland. He entered the School of Engineering Air Force Institute of Technology in August 1979.

Permanent Address: 700 Lenox Avenue
New York, NY 10039

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Finite Elements

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A finite element space-angle synthesis solution of the steady state ani[so]tropic Boltzmann (transport) equation in a two-dimensional cylindrical geome[try] has been developed. Starting from a variational principle, the Bubnov-Galer[kin] solution method was applied to the second order even parity form of the Boltzmann equation. A trial function flux expansion in bicubic splines and spherical (surface) harmonics was used. A first scatter (collision) source [for] an exponentially varying atmosphere was also incorporated into this developm[ent].

(Continued on Reverse)

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BLOCK 20: ABSTRACT (Cont'd)

Finite element space-angle synthesis (FESAS) was developed as an alternate solution approach and an improvement in comparison to the methods of Monte Carlo and discrete ordinates. FESAS does not have the inherent characteristics which have produced the ray effect problem in discrete ordinates. Also, FESAS may result in lower computational costs than those of Monte Carlo and discrete ordinates.

The second order even parity form of the Boltzmann equation was derived and shown to be symmetric, positive definite and self-adjoint. The equivalence of a variational minimization principle and the Bubnov-Galerkin method of weighted residuals was established. The finite element space angle synthesi system of equations was expanded and a numerical computer solution approach was implemented. A computer program was written to solve for the trial function expansion (mixing) coefficients, and also to compute the particle flux.

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